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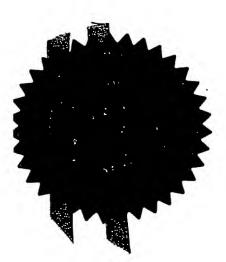
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METHODS

The present invention relates to protein kinase catalytic domain structures and mutants and screening assays making use thereof.

The 3-Phosphoinositide Dependent Protein Kinase-1 (PDK1) is a key protein kinase, regulating activity of a group of related protein kinases through phosphorylation. These kinases include isoforms of Protein Kinase B (also known as Akt) [Brazil and Hemmings, 2001, Scheid and Woodgett, 2001], p70 ribosomal S6 kinase (S6K) [Alessi et al., 1997, Volarevic and Thomas, 2001], p90 ribosomal S6 Kinase (RSK) [Frodin and Gammeltoft, 1999] and the serum and glucocorticoid induced-protein kinase (SGK) [Lang and Cohen, 2001]. These enzymes are stimulated by hormones and growth factors and phosphorylate regulatory proteins mediating the various physiological effects of these agonists.

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PDK1 possesses an N-terminal kinase catalytic domain and a C-terminal pleckstrin homology (PH) domain [Alessi et al., 1997, Stephens et al., 1998]. PDK1 activates its substrates by phosphorylating these kinases at their activation loop (reviewed in [Alessi, 2001, Toker and Newton, 2000]). The phosphorylation of PKB by PDK1 is dependent upon prior activation of the phosphoinositide 3-kinase (PI-3-kinase) and the production of the second messenger, phosphatidylinositol 3,4,5-trisphosphate (PtdIns(3,4,5)P₃) which binds to the PH domains of PDK1 and PKB. This does not activate either PKB or PDK1 but instead recruits and co-localises these enzymes at the plasma membrane.

Unlike PKB, the other PDK1 substrates described thus far do not interact with PtdIns(3,4,5)P₃ nor is the rate at which they are phosphorylated by PDK1 further enhanced by the binding of PDK1 to PtdIns(3,4,5)P₃. Instead the ability of PDK1 to phosphorylate S6K, SGK and RSK is promoted by

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phosphorylation of these enzymes at a residue located C-terminal to the kinase catalytic domain in a region known as the hydrophobic motif [Alessi et al., 1997,Kobayashi and Cohen, 1999, Pullen et al., 1998]. The kinases that phosphorylate the hydrophobic motif of S6K and SGK are unknown but as the phosphorylation of this residue *in vivo* is dependent on PI-3-kinase activation, the hydrophobic motif kinases and/or the hydrophobic motif phosphatases may be regulated by PtdIns(3,4,5)P₃. In the case of RSK isoforms, phosphorylation by the ERK1/ERK2 MAP kinases induce phosphorylation of the hydrophobic motif (reviewed in Frodin and Gammeltoft, 1999).

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PDK1 belongs to the same subfamily of protein kinases as its substrates, termed the AGC protein kinases as they are related to the cAMP dependent protein kinase (PKA)/cGMP dependent protein kinase/Protein kinase C (PKC). PKA is the only AGC kinase whose crystal structure has been solved. Like all protein kinases, its catalytic core possesses an N-terminal lobe consisting mainly of β -sheet and a predominantly α -helical Cterminal lobe [Taylor et al., 1992, Husen and Kuriyan, 2002]. The ATP binding site is located in between the 2 lobes [Johnson et al., 2001, Knighton et al., 1991]. At the very C-terminus, PKA possesses an extended loop that terminates in the sequence FXXF which resembles the first part of the hydrophobic motif phosphorylation site of S6K and SGK (FXXFS/TY) in which the Ser/Thr is the phosphorylated residue [Biondi et al., 2000]. In the structure of PKA, the FXXF motif is buried in a hydrophobic pocket in the small lobe of the PKA catalytic domain [Knighton et al., 1991] and mutation of either of the Phe residues drastically reduces PKA activity towards a peptide substrate [Etchebehere et al., 1997]. Unlike other AGC kinases, PDK1 does not possess a hydrophobic motif C-terminal to its catalytic domain. However, there is evidence that PDK1 possesses a hydrophobic pocket in the small lobe of its catalytic domain similar to that

in PKA. We have biochemically demonstrated that the interaction of PDK1 with four of its substrates (S6K1, SGK1, PKζ and PKC related kinase-2 (PRK2)) is reduced or abolished by mutation of residues predicted to form part of this pocket [Balendran et al., 2000, Biondi et al., 2000]. Furthermore, mutation of a central residue in the predicted pocket, Leu 155, prevented PDK1 from phosphorylating and activating S6K1 and SGK1 without affecting its ability to phosphorylate either PKB or a short peptide substrate that encompasses the activation loop of PKB (T308tide) [Biondi et al., 2000]. The hydrophobic pocket on the kinase domain of PDK1 has been termed the "PIF-pocket" after the name of the first AGC-kinase hydrophobic motif-containing peptide (PDK1 Interacting Fragment) that was found to bind PDK1 [Balendran et al., 1999a]. It has been suggested that the PIF-pocket in PDK1 functions as a docking site, enabling PDK1 to interact with some of its.physiological substrates. Furthermore, there is evidence that phosphorylation of the hydrophobic motif of S6K1, SGK and RSK2 [Balendran et al., 1999b, Biondi et al., 2001, Frodin et al., 2000] promotes the interaction of these enzymes with PDK1. These findings suggest that the PIF-pocket on PDK1 could contain a phosphate binding site promoting the binding of PDK1 to a subset of substrates (S6K, SGK and RSK) once these enzymes have been phosphorylated at their hydrophobic motif. This would result in a physiological phosphate dependent interaction. In addition there is evidence that occupancy of the PIF-pocket activates PDK1 as peptides that encompass the hydrophobic motif of PRK2 [Biondi et al., 2000] and RSK [Frodin et al., 2000] induce a 4-6-fold activation of PDK1.

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Previous predicted structures PDK1 catalytic domain were obtained using homology modelling methods based upon structural information available from the catalytic domain of PKA (Biondi et al., 2000). These predictions of the PDK1 catalytic domain structure were thus biased towards the catalytic domain from which the structural information was obtained.

We have determined a crystal structure for the kinase domain of the AGC family protein kinase PDK. The structure defines the PIF-pocket and reveals an adjacent possible phosphate binding site. Furthermore, we have performed structure-based mutagenesis and biochemical analysis which support the existence of such a phosphate-binding site. This may mediate the phosphate dependent docking interaction with substrates such as (for PDK1) S6K and SGK. We have used a novel algorithm to define the conformational state of the crystallised PDK1 relative to all the reported structures of PKA, which shows that while PDK1 has all the signs of being in an active form in the crystal, its overall conformation is in-between and 'open' and 'closed' state. On the basis of this work we provide drug screening methods and mutated protein kinase molecules (which are useful in, for example, drug screening methods).

A first aspect of the invention provides a method for selecting or designing a compound for modulating the activity of phosphoinositide dependent protein kinase 1 (PDK1), the method comprising the step of using molecular modelling means to select or design a compound that is predicted to interact with the protein kinase catalytic domain of PDK1, wherein a three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 is compared with a three-dimensional structure of a compound, and a compound that is predicted to interact with the said protein kinase catalytic domain is selected, wherein the three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 is a three-dimensional structure (or part thereof) determined for a polypeptide consisting of residues equivalent to residues 51 to 359 of full length human PDK1, or a fragment or fusion thereof.

The term PDK1 as used herein includes a polypeptide (a PDK1 polypeptide) comprising the amino acid sequence identified as PDK1 in Alessi D.R et al (1997) Curr. Biol. 7: 261-269, Alessi D.R et al (1997) Curr. Biol. 7: 776-789, Stokoe D et al (1997) Science 277: 567-570 or Stephens L et al (1998) Science 279: 710-714, or a variant, fragment, fusion or derivative thereof, or a fusion of a said variant or fragment or derivative, for example as described in WO98/41638, incorporated herein by reference. It is preferred that the said PDK1 polypeptide is a protein kinase. It is preferred that the said PDK1 polypeptide is a protein kinase that is capable of phosphorylating a threonine residue that lies in a Thr-Phe-Cys-Gly-Thr-10 Xaa-Glu-Leu consensus motif (where the underlined Thr corresponds to the threonine that is phosphorylated by PDK1 and Xaa is a variable residue), and preferably that is capable of phosphorylating PKB, for example PKBa, at residue Thr308. The rate at which the said PDK1 polypeptide is capable of phosphorylating a threonine residue as described above may be increased 15 in the presence of PtdIns(3,4,5)P₃ or PtdIns(3,4)P₂ but it will be appreciated that this is not essential. The said polypeptide may be capable of phosphorylating the equivalent residues to Thr308 of PKB α on PKC isoforms (LeGood et al (1998) Science 281: 2042-2045; et al (1998) Curr. Biol. 8: 1069-1077; Dutil et al (1998) Curr. Biol. 8:1366-1375), p70 S6 20 kinase (Alessi et al (1998) Curr. Biol. 8: 69-81; Pullen et al (1998) Science 279, 707-710), SGK (sequence given in Webster et al (1993) Mol. Cell. Biol. 13, 1031-2040; equivalent residues identified in US application no 112217 filed on 14 December 1998; GB 9919676.8, filed on 19 August 1999, and Kobayashi & Cohen (1999)) and PKA (Cheng et al (1998) Proc. 25 Natl. Acad. Sci. USA 95: 9849-9854). It may further be preferred that the substrate specificity and/or other characteristics of the said PDK1 polypeptide in vitro may be substantially as reported in Alessi D.R et al (1997) Curr. Biol. 7: 261-269, Alessi D.R et al (1997) Curr. Biol. 7: 776789, Stokoe D et al (1997) Science 277: 567-570 or Stephens L et al (1998) Science 279: 710-714.

We have found that a fragment of PDK1 consisting essentially of residues equivalent to residues 51 to 359 of full length human PDK1 is particularly beneficial for determining a structure for the catalytic domain of PDK1. This fragment has, for example, protein kinase activity and surprisingly beneficial solubility and stability characteristics which make it particularly suitable for structural studies, for example formation of crystals which may be analysed by X-ray crystallography methods. Other fragments of PDK1 were surprisingly found to be unsuitable for crystallisation, as discussed in Example 5.

It is particularly preferred that the structure is one determined for the fragment consisting of residues 51 to 359 of full length human PDK1. The fragment may comprise an N-terminal or C-terminal fusion polypeptide (ie amino acid sequence not derived from PDK1), though this is preferably of less than or equal to about 10, 5, 4, 3, 2 or 1 amino acids. For example, it is particularly preferred that the structure is one determined for a polypeptide consisting residues 51 to 359 of full length human PDK1 and the amino acid sequence Gly-Pro (or less preferably other sequence forming part of a protease cleavage site) preceding the methionine corresponding to Met51 of human PDK1. A further preferred structure is one determined for the fragment consisting essentially of residues 71 to 359 of full length human PDK1 (or residues equivalent thereto), which also has protein kinase activity.

It is particularly preferred that the structure is one determinable by a method as described in Example 1, for example a structure obtainable by X-ray analysis from a crystal obtainable using a mother liquor solution comprising

ammonium sulphate, preferably between 1.8 and 2.2M. It is particularly preferred that the mother liquor solution is of pH 7 to 9, preferably 7 to 8.5, most preferably pH8.5, and comprises ammonium sulphate and preferably ATP. Crystals may form in the absence of ATP but better crystals may be obtained in the presence of ATP. Preferably the crystal is obtainable using a mother liquor solution containing 0.1M Tris/HCl pH 8.5, 2.0 M ammonium sulphate, 16.6 mM ATP. Further preferred details of the crystallisation and X-ray analysis are described in Example 1, for example as partially summarised in Table 1 (shown in Example 1).

It is particularly preferred that the structure is that represented by the structure co-ordinates shown in Examples 2, 3 or 4, or a structure based or modelled on such a structure or co-ordinates. The co-ordinates shown in Example 2 are for the PDK1 fragment with all alternate side chains. The co-ordinates shown in Example 3 are for the PDK1 fragment without alternate side chains. The co-ordinates shown in Example 4 are for the dimer of the PDK1 fragment, without alternate side chains; chain A is the molecule for which co-ordinates are given in Examples 2 and 3, and chain B is the symmetry-related molecule.

It is preferred that the molecule is predicted to bind to a region of the structure termed the "PIF binding pocket", the "phosphate binding pocket" and/or the α C helix (residues equivalent to 123-136 of full length human PDK1), particularly the residue equivalent to Arg 131 of full length human PDK1, or interacting regions. As discussed in Example 1, the PIF binding pocket is considered to be formed by residues including Lys115, Ile118, Ile119 on the α B helix, Val124, Val127 on the α C helix and Leu 155 on β -sheet 5. The phosphate binding pocket is considered to be formed by residues including Lys76, Arg 131, Thr 148 and Gln150. Residues of the α C helix that are considered to interact either with phosphate bound in the

phosphate binding site or intermolecularly with phosphorylated Ser241 of PDK1 include Arg131 (phosphate binding site) and Arg 129 and His126 (phosphorylated Ser241). Glu 130 is involved in binding the α-phosphate of the bound ATP, and Val124 and Val127 form part of the PIF binding pocket, as discussed in Example 1.

It is preferred that the compound is for modulating the protein kinase activity of PDK1. The protein kinase activity of PDK1 that is modulated may be phosphorylation of the underlined residue in a polypeptide with the amino acid sequence Thr/Ser-Phe-Cys-Gly-Thr-Xaa-Glu-Leu ("PDK1" activity). Alternatively or in addition, the modulated activity may be phosphorylation of the underlined residue in a polypeptide with the amino acid sequence Phe-Xaa-Xaa-Phe-Ser/Thr-Phe/Tyr ("PDK2" activity). The substrate polypeptide may be, for example, a PKB, SGK, p70 S6 kinase, PKC or (in relation only to phosphorylation of the underlined residue in a polypeptide with the amino acid sequence Thr/Ser-Phe-Cys-Gly-Thr-Xaa-Glu-Leu) PKA polypeptide. The modulated protein kinase activity may be towards PKB or other PH-domain-comprising/phosphoinositide-binding substrate of PDK1; or SGK, S6K or other substrate of PDK1 whose phosphorylation by PDK1 is promoted by phosphorylation of the substrate on the Ser/Thr of the "hydrophobic motif' FXXFS/TY; or an artificial substrate such as T308tide (which comprises the sequence of PKB which is phosphorylated by PDK1) or PDKtide (which comprises the sequence of PKB which is phosphorylated by PDK1 (eg T308tide) fused to a sequence mimicking a phosphorylated hydrophobic motif ie FXXFZY, in which Z is a negatively charged (for example acidic) residue (eg PIFtide)). substrates for PDK1 are discussed, for example, in WO 01/44497. Other activities of PDK1 that may be modulated include interactions with other polypeptides or phosphoinositides and/or intramolecular interactions.

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It is preferred that the three-dimensional structure of at least a part of the protein kinase catalytic domain of the PDK1 is a three-dimensional structure of at least a part of the PIF binding pocket, the phosphate binding pocket and/or the α C helix, or interacting regions of PDK1, and a compound that is predicted to interact with the said PIF binding pocket, the phosphate binding pocket and/or the α C helix, or interacting regions of PDK1 is selected. Alternatively, the compound may bind to a portion of said PDK1 polypeptide that is not the PIF binding pocket, the phosphate binding pocket and/or the α C helix, or interacting regions of PDK1, for example so as to interfere with the binding of the ATP or substrate polypeptide or their access to the catalytic site. In a still further example, the compound may bind to a portion of PDK1 so as to decrease said polypeptide's activity by an allosteric effect. This allosteric effect may be an allosteric effect that is involved in the natural regulation of PDK1's activity.

It is further preferred that the three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 is a three-dimensional structure of the part of the protein kinase catalytic domain of PDK1 that is defined by residues Lys115, Ile118, Ile119 (on the αB helix), Val124, Val127 (on the αC helix) and Leu 155 (on β -sheet 50 and/or residues Lys76, Arg 131, Thr 148 and Gln150 and/or residues Arg131, Arg 129, His126, Glu 130 of full-length human PDK1 and a compound that is predicted to interact with the said part of the protein kinase catalytic domain is selected.

For example, it is preferred if the portions of the structure of PDK1 shown in Figures 1 and 2 as forming the PIF binding pocket and/or phosphate binding pocket and/or αC helix interactions (for example with

phosphoserine241) are compared with the structure of the candidate compound.

A further aspect of the invention provides a method for selecting or designing a compound for modulating the activity of a hydrophobic pocket (PIF binding pocket)-containing protein kinase having a hydrophobic pocket in the position equivalent to the hydrophobic pocket of human PDK1 that is defined by residues including Lys115, Ile118, Ile119, Val124, Val127 and/or Leu155 of full-length human PDK1 and further having a phosphate binding pocket in the position equivalent to the phosphate binding pocket of human PDK1 that is defined by residues including Lys76, Arg131, Thr148 and/or Gln150, the method comprising the step of using molecular modelling means to select or design a compound that is predicted to interact with the said hydrophobic pocket-containing protein kinase. wherein a three-dimensional structure of a compound is compared with a three-dimensional structure of the said phosphate binding pocket and optionally also the hydrophobic pocket and/or aC helix or region interacting therewith, and a compound that is predicted to interact with the said phosphate binding pocket and optionally also the hydrophobic pocket and/or aC helix or region interacting therewith, is selected.

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The three-dimensional structure of a compound may be compared with the three-dimensional structure of the hydrophobic and/or phosphate binding pocket and/or αC helix or region interacting therewith, as appropriate. A compound that can interact with the hydrophobic pocket and/or phosphate binding pocket, in particular residues noted above as defining such regions, in a similar manner (for example similar separation and/or type of interaction ie hydrophobic or ionic, and/or similar cumulative energy of interaction) to an interacting polypeptide such as S6K-pHM may be

selected. Methods of assessing the interaction are well known to those skilled in the art and are discussed further below.

The three-dimensional structures that are compared may be, as appropriate, predicted or modelled three-dimensional structures (for example on the basis of a PDK1 structure as referred to above, for example as represented by the co-ordinates given in Examples 2, 3 or 4) or may be three-dimensional structures that have been determined, for example by techniques such as X-ray crystallography, as well known to those skilled in the art. The three-dimensional structures may be displayed by a computer in a two-dimensional form, for example on a computer screen. The comparison may be performed using such two-dimensional displays.

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The following relate to molecular modelling techniques: Blundell *et al* (1996) Stucture-based drug design *Nature* 384, 23-26; Bohm (1996) Computational tools for structure-based ligand design *Prog Biophys Mol Biol* 66(3), 197-210; Cohen *et al* (1990) *J Med Chem* 33, 883-894; Navia *et al* (1992) *Curr Opin Struct Biol* 2, 202-210.

The following computer programs, for example, may be useful in carrying out the method of this aspect of the invention: GRID (Goodford (1985) J Med Chem 28, 849-857; available from Oxford University, Oxford, UK); MCSS (Miranker et al (1991) Proteins: Structure, Function and Genetics 11, 29-34; available from Molecular Simulations, Burlington, MA); AUTODOCK (Goodsell et al (1990) Proteins: Structure, Function and Genetics 8, 195-202; available from Scripps Research Institute, La Jolla, CA); DOCK (Kuntz et al (1982) J Mol Biol 161, 269-288; available from the University of California, San Francisco, CA); LUDI (Bohm (1992) J Comp Aid Molec Design 6, 61-78; available from Biosym Technologies, San Diego, CA); LEGEND (Nishibata et al (1991) Tetrahedron 47, 8985;

available from Molecular Simulations, Burlington, MA); LeapFrog (available from Tripos Associates, St Louis, MO); Gaussian 92, for example revision C (MJ Frisch, Gaussian, Inc., Pittsburgh, PA ©1992); AMBER, version 4.0 (PA Kollman, University of California at San Francisco, ©1994); QUANTA/CHARMM (Molecular Simulations, Inc., Burlington, MA ©1994); and Insight II/Discover (Biosym Technologies Inc., San Diego, CA ©1994). Programs may be run on, for example, a Silicon GraphicsTM workstation, Indigo²TM or IBM RISC/6000TM workstation model 550.

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Several *in silico* methods could be employed, for example, via a substructure search for new ligands using programmes such as CHEM DRAW or CHEM FINDER. The basic structure of the natural ligand (for example a phosphorylated hydrophobic motif peptide such as S6K-pHM) capable of binding to PDK1 (or other protein kinase) is taken (or predicted) and various structural features of it (for example the hydrophobic and negatively charged entities) are submitted to a programme which will searches a set of chemical company catalogues for chemicals containing this substructure.

These compounds are then screened by eye for groups that could not interact with the PIF/phosphate binding pockets (or the αC residues/interacting region) because, for example, they are too large or have steric or charge hindrance, and those are discarded. The remaining chemicals are submitted to a PRODRG server and topologies/co-ordinates for these chemicals are created. These chemicals are modelled into the structure, from which chemicals that are possibly able to bind to the PIF/phosphate binding site domain/αC helix/interacting region are selected. Further details of the PRODRG programme are available at http://davapc1.bioch.dundee.ac.uk/programs/prodrg/prodrg.html.

These compounds may then be ordered or synthesised and assessed, for one or more of ability to bind to and/or modulate PDK1 (or other protein kinase) activity. The compounds may be crystallised with the PDK1 or other protein kinase protein and the structure of any complex determined.

An alternative approach is to use PRODRG: a tool for generating GROMOS/MOL2/WHATIF topologies and hydrogen atom positions from small molecule PDB files. We take the natural ligand and computationally vary all possible groups at each site on the ligand, with a variety of new groups while the protein co-ordinates and the ligand back-bone co-ordinates remain fixed the results can then be screened for hindrance and repulsion, and the molecules are obtained either through catalogues or made.

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As noted above, the selected or designed compound may be synthesised (if not already synthesised) or purified and tested for its effect on the relevant hydrophobic/phosphate pocket-containing protein kinase, for example its effect on the protein kinase activity. The compound may be tested in a screening method of the invention or other screening method. The compound may be formulated for pharmaceutical use, for example for use in *in vivo* trials in animals or humans, or for use in agriculture, for example as an antifungal agent.

It may be useful to analyse a protein kinase structure (for example a structure determined or predicted for a complex of the protein kinase with a binding partner) in order to determine the activation state of the structure. This may be useful in further modelling binding of the binding partner to the protein kinase in other activation states, and in predicting how the binding partner may affect the activation state of the protein kinase or compete with other potential binding partners. It may also be useful in designing and assessing derivatives of the binding partner.

Thus, a further aspect of the invention provides a method for assessing the activation state of a structure for a protein kinase, wherein the structure is analysed using principle component analysis of the structure co-ordinates. The method may further comprise the step of classifying the activation state of the structure as "open", "closed" or "intermediate". Details of the analysis, which involves the generation of eigenvectors and associated eigenvalues are given in Example 1. The analysis makes use of techniques described in Amadei et al (1993) Essential dynamics of proteins. Proteins 17, 412-425.

The hydrophobic/phosphate pocket-containing protein kinase may be PDK1. Alternatively, it may be an isoform of Serum and Glucocorticoid stimulated protein kinase (SGK), Protein Kinase B (PKB), p70 S6 kinase, p90 RSK, PKC isoforms (for example PKCα, PKCδ, PKCζ), PRK1, PRK2, MSK1 or MSK2. Hydrophobic/phosphate pocket-containing protein kinases and their EMBL database accession numbers are listed in Table I. Sequences considered to form the phosphate binding pocket from representative hydrophobic/phosphate pocket-containing protein kinases are shown in Figure 5. All AGC family protein kinases other than PKA may be hydrophobic/phosphate pocket-containing protein kinases, as defined above. In addition to the protein kinases shown in Figure 7, rhodopsin and G-protein coupled receptor protein kinases, for example, may possibly also have a hydrophobic/phosphate pocket as defined above.

The terms SGK, PKB, p70 S6 kinase, p90 RSK, PKCα, PKCδ, PKCζ or PRK2, for example, as used herein include a polypeptide (a SGK, PKB, PKA, p70S6 kinase, p90 RSK, PKCα, PKCδ, PKCζ or PRK2 polypeptide) comprising the amino acid sequence identified as a SGK, PKB, p70 S6

kinase, p90 RSK, PKCα, PKCδ, PKCζ or PRK2, respectively, in the relevant EMBL database records indicated in Table 2.

Table 2

	Activation or I	T- AGC	Accession
	Loop	Hydrophobic	number
		Motif	•
consensus:	$\underline{\mathtt{T}}\mathtt{FCGTxxYxAPD}$	FxxF <u>S</u> Y	
	L E	$Y\underline{\mathbf{T}}\mathbf{F}$	
PKBα	$\underline{\mathtt{T}}$ FCGTPEYLAPE	FPQF <u>S</u> Y	(Y15056)
РКВβ	$\underline{\mathtt{T}}$ FCGTPEYLAPE	FPQF <u>S</u> Y	(P31751)
ΡΚΒγ	TFCGTPEYLAPE	FPQF <u>S</u> Y	(AF135794)
SGK1	TFCGTPEYLAPE	FLGFSY	(AAD41091)
SGK2	$\underline{\mathtt{T}}\mathtt{FCGTPEYLAPE}$	$\mathtt{FLGF}\underline{\mathtt{S}}\mathtt{Y}$	(AF169034)
SGK3	<u>T</u> FCGTPEYLAPE	$\mathtt{FLGF}\underline{\mathtt{S}}\mathtt{Y}$	(AF169035)
PKCα	<u>T</u> FCGTPDYIAPE	FEGF <u>S</u> Y	(4506067)
РКСβІ	TFCGTPDYIAPE	FAGF <u>S</u> Y	(4506069)
РКСВП	$\underline{\mathtt{T}}\mathtt{FCGTPDYIAPE}$	FEGF <u>S</u> F	(P05127)
РКСү	$\underline{\mathtt{T}}\mathtt{FCGTPDYIAPE}$	$\mathtt{FGGF}\underline{\mathtt{T}}\mathtt{Y}$	(P05129)
РКСδ	TFCGTPDYIAPE	fagf <u>s</u> f	(5453970)
PCKζ _.	$\underline{\mathtt{T}}$ FCGTPNYIAPE	FEGFEY	(4506079)
PKCı	$\underline{\mathtt{T}}\mathtt{FCGTPNYIAPE}$	FEGFEY	(4506071)
PRK1	$\underline{\mathtt{T}}\mathtt{FCGTPEFLAPE}$	FLDFDF	(AAC50209)
PRK2	$\underline{\mathtt{T}}\mathtt{FCGTPEFLAPE}$	FRDFDY	(AAC50208)
p70-S6 $K\alpha$	$\underline{\mathtt{T}}\mathtt{FCGTIEYMAPE}$	$\mathtt{FLGF}\underline{\mathtt{T}}\mathtt{Y}$	(AAA36410)
p70-S6Kβ	$\underline{\mathtt{T}}\mathtt{FCGTIEYMAPE}$	FLGF <u>T</u> Y	(4506739)
p90-RSK1	<u>S</u> FCGTVEYMAPE	FRGF <u>S</u> F	(138556)
p90-RSK2	<u>S</u> FCGTVEYMAPE	FRDF <u>S</u> F	(P51812)
p90-RSK3	<u>S</u> FCGTIEYMAPE	FRGF <u>S</u> F	(CAA59427)

MSK1	SFCGTIEYMAPD	FQGY <u>S</u> F	(AAC31171)
MSK2	<u>S</u> FCGTIEYMAPE	FQGY <u>S</u> F	(AAC67395)
PDK1	<u>S</u> FVGTAQYVSPE	(1)	(AF017995)

Table 2. Alignment of the amino acid sequences surrounding the T-loop and the hydrophobic motif of AGC kinases. All the sequences and accession numbers are from human proteins. The underlined residues correspond to those that become phosphorylated. Footnotes: (1) PDK1 does not possess a hydrophobic motif.

It is preferred that the PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase) is a polypeptide which consists of the amino acid sequence of the protein kinase PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase as the case may be) sequence referred to above or naturally occurring allelic variants thereof. It is preferred that the naturally occurring allelic variants are mammalian, preferably human, but may alternatively be homologues from parasitic or pathogenic or potentially pathogenic organisms. Examples of such organisms and homologues, and of uses of modulators of such homologues are given in US patent application No 60/112,114, filed on 14 December 1998, and applications claiming priority therefrom, or in Casamayor et al (1999) Curr Biol 9, 186-197.

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The PDK1 may also be a polypeptide with the amino acid sequence of residues 51 to 359 or 404 (or 71 to 360) of full-length human PDK1; this may comprise the protein kinase domain of PDK1, as described in Example 2. The PDK1 (or SGK, PKB, PKA or p70 S6 kinase) may also be Myc epitope-tagged or His-tagged, as described in Example 1. The p70 S6 kinase, for example, may have a His tag at its N-terminus and/or may lack the carboxy terminal 104 residues (p70 S6K-T2). The PDK1 or SGK may

be a Saccharomyces cerevisiae homologue, for example Pkh1 or Pkh2 (PDK1 homologues) or Ypk1 or Yrk2 (SGK homologues), as described in Casamayor et al (1999) Curr Biol 9, 186-197.

It is particularly preferred, although not essential, that the variant or 5 fragment or derivative or fusion of the PDK1, or the fusion of the variant or fragment or derivative has at least 30% of the enzyme activity of full-length human PDK1 with respect to the phosphorylation of full-length human PKBa on residue Thr308 or SGK1 on residue Thr 256 in either the presence or absence of PtdIns(3,4,5)P₃ or PtdIns(3,4)P₂. It is more preferred if the 10 variant or fragment or derivative or fusion of the said protein kinase, or the fusion of the variant or fragment or derivative has at least 50%, preferably at least 70% and more preferably at least 90% of the enzyme activity of PDK1 with respect to the phosphorylation of PKBa or SGK1. However, it will be appreciated that variants or fusions or derivatives or fragments which are devoid of enzymatic activity may nevertheless be useful, for example by interacting with another polypeptide. Thus, variants or fusions or derivatives or fragments which are devoid of enzymatic activity may be useful in a binding assay, which may be used, for example, in a method of the invention in which modulation of an interaction of a mutated PDK1 of the invention and optionally also PDK1 with a interacting polypeptide or compound, for example an interacting polypeptide comprising the amino acid sequence motif Phe/Tyr-Xaa-Xaa-Phe/Tyr, for example Phe/Tyr-Xaa-Xaa-Phe/Tyr-Zaa-Phe/Tyr, for example Phe/Tyr-Xaa-Xaa-Phe/Tyr-Asp/Glu-Phe/Tyr or Phe/Tyr-Xaa-Xaa-Phe/Tyr-PhosphoSer/PhosphoThr-Phe/Tyr is measured.

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It is preferred that the variant or fragment or derivative or fusion of the said hydrophobic/phosphate binding pocket-containing protein kinase, or the fusion of the variant or fragment or derivative comprises a hydrophobic

pocket and a phosphate binding pocket in the position equivalent to the hydrophobic and phosphate binding pocket of human PDK1, as discussed further below.

Equivalent preferences apply to a variant or fragment or derivative or fusion of the SGK, PKB, p70 S6 kinase, p90 RSK, PKCα, PKCδ, PKCζ or PRK2 (for example), or the fusion of the variant or fragment or derivative, with the substitution in relation to SGK, PKB and p70S6 kinase of the peptide substrate Crosstide (GRPRTSSFAEG), or for PKB and SGK of the peptide substrate RPRAATF; the substitution in relation to PKA of the peptide substrate Kemptide (LRRASLG); the substitution in relation to PKC isoforms and PRK1/2 of histone H1; and the substitution in relation to MSK1/2 or p90-RSK1/2/3 of CREBtide (EILSRRPSYRK).

15 By "variants" of a polypeptide we include insertions, deletions and substitutions, either conservative or non-conservative. In particular we include variants of the polypeptide where such changes do not substantially alter the activity of the said polypeptide, for example the protein kinase activity of PDK1, as described above.

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By "conservative substitutions" is intended combinations such as Gly, Ala; Val, Ile, Leu; Asp, Glu; Asn, Gln; Ser, Thr; Lys, Arg; and Phe, Tyr.

The three-letter amino acid code of the IUPAC-IUB Biochemical Nomenclature Commission is used herein, with the exception of the symbol Zaa (negatively charged amino acid). In particular, Xaa represents any amino acid. It is preferred that Xaa and Zaa represent a naturally occuring amino acid. It is preferred that at least the amino acids corresponding to the consensus sequences defined above are L-amino acids.

It is particularly preferred if the PDK1 (or SGK, PKB, PKA or p70 S6 kinase or other hydrophobic/phosphate binding pocket-containing kinase as defined above) variant has an amino acid sequence which has at least 65% identity with the amino acid sequence of PDK1 referred to above (or the sequence for SGK (including SGK1, 2 and 3), PKB, PKA or p70 S6 kinase, for example, as appropriate, referred to above), more preferably at least 70%, 71%, 72%, 73% or 74%, still more preferably at least 75%, yet still more preferably at least 85%, in still further preference at least 80% in further preferably at least 95% or 97% identity with the amino acid sequence defined above.

It is still further preferred if the PDK1 (or SGK, PKB, PKA or p70 S6 kinase or other hydrophobic/phosphate binding pocket-containing kinase, as defined above) variant has an amino acid sequence which has at least 65% identity with the amino acid sequence of the catalytic domain, particularly the residues forming the hydrophobic pocket, of PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase) in the appropriate sequence referred to above, more preferably at least 70%, 71%, 72%, 73% or 74%, still more preferably at least 75%, yet still more preferably at least 80%, in further preference at least 83 or 85%, in still further preference at least 90% and most preferably at least 95% or 97% identity with the amino acid sequence defined above. It will be appreciated that the catalytic domain of a protein kinase-related polypeptide may be readily identified by a person skilled in the art, for example using sequence comparisons as described below.

The percent sequence identity between two polypeptides may be determined using suitable computer programs, for example the GAP program of the University of Wisconsin Genetic Computing Group and it will be appreciated that percent identity is calculated in relation to polypeptides whose sequence has been aligned optimally.

The alignment may alternatively be carried out using the Clustal W program (Thompson *et al* (1994) *Nucl Acid Res* 22, 4673-4680). The parameters used may be as follows:

Fast pairwise alignment parameters: K-tuple(word) size; 1, window size; 5, gap penalty; 3, number of top diagonals; 5. Scoring method: x percent.

Multiple alignment parameters: gap open penalty; 10, gap extension penalty; 0.05.

Scoring matrix: BLOSUM.

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It is preferred that the PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase) is a polypeptide which consists of the amino acid sequence of the protein kinase PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase as the case may be) sequence referred to above or naturally occurring allelic variants thereof. It is preferred that the naturally occurring allelic variants are mammalian, preferably human, but may alternatively be homologues from parasitic or pathogenic or potentially pathogenic organisms. Examples of such organisms and homologues, and of uses of modulators of such homologues are given in US patent application No 60/112,114, filed on 14 December 1998, and applications claiming priority therefrom, or in Casamayor et al (1999) Curr Biol 9, 186-197.

It is preferred that the PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase) is a polypeptide that is capable of interacting with a polypeptide comprising the amino acid sequence motif Phe/Tyr-Xaa-Xaa-Phe/Tyr, preferably Phe-Xaa-Xaa-Phe/Tyr, more preferably Phe-Xaa-Xaa-Phe, still more preferably Phe/Tyr-Xaa-Xaa-Phe/Tyr-Zaa-Phe/Tyr-Zaa-Phe/Tyr-Xaa-Xaa-Phe/Tyr-COOH, for example the polypeptide PIF or PIFtide, as defined below. Further preferences for the said polypeptide are as given above.

The protein kinase activity of PKB, SGK or p70 S6 kinase that is modulated may be phosphorylation of the underlined residue in a polypeptide with the amino acid sequence Arg-Xaa-Arg-Xaa-Xaa-Ser/Thr. The polypeptide may be Glycogen Synthase Kinase 3 (GSK3), 40 S ribosomal subunit S6, BAD, 6-phosphofructo-2-kinase, phosphodiesterase3b, human caspase 9, endothelial nitric oxide synthase or BRCA1.

A compound identified by a method of the invention may modulate the ability of the protein kinase to phosphorylate different substrates, for example different naturally occurring polypeptides, to different extents. The compound may inhibit the protein kinase activity in relation to one substrate but may increase the protein kinase activity in relation to a second substrate. For example, the protein kinase activity of PDK1 may be modulated to a different extent for PKB when compared with SGK, p70 S6 kinase and/or PKC.

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It will be appreciated that the modulatory, for example inhibitory action of a compound found to bind (or inhibit binding of a polypeptide or compound) to the protein kinase may be confirmed by performing an assay of enzymic activity (for example PDK1 and/or PDK2 protein kinase activity) in the presence of the compound.

By "hydrophobic pocket-containing protein kinase having a hydrophobic pocket (PIF binding pocket) in the position equivalent to the hydrophobic pocket of human PDK1 that is defined by residues including Lys115, Ile118, Ile119, Val124, Val127 and/or Leu155 of full-length human PDK1 and further having a phosphate binding pocket in the position equivalent to the phosphate binding pocket of human PDK1 that is defined by residues including Lys76, Arg131, Thr148 and/or Gln150," is meant a polypeptide

having an amino acid sequence identifiable as that of a protein kinase catalytic domain, and further having a predicted or determined three-dimensional structure that includes a hydrophobic pocket corresponding to the region indicated in Example 1 as the PIF binding pocket, and a pocket corresponding to the region indicated in Example 1 as the phosphate binding pocket. The hydrophobic pocket and phosphate binding pockets in PDK1 do not overlap with the ATP or phosphorylation site binding sites on PDK1.

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It is preferred that the protein kinase has identical or conserved residues that are equivalent to Lys 115, Ile118, Ile119, Val124, Val127 and/or Leu 155 of human PDK1, more preferably at least Lys115 and Leu155 of human PDK1, most preferably an identical residue equivalent to Leu155. Thus, for example, the protein kinase may have a Lys residue at the position equivalent to Lys115 of PDK1 and/or a Leu residue at the position equivalent to Leu155 of PDK1. It is preferred that the protein kinase does not have an Ala at the position equivalent to Lys115 and/or a Ser, Asp or Glu at the position equivalent to Leu155 of PDK1.

It is further preferred that the protein kinase has identical or conserved residues that are equivalent to Lys76, Arg131, Thr148 and/or Gln 150 of human PDK1, more preferably at least Lys76 and Gln150 of human PDK1, most preferably an identical residue equivalent to Gln150. Figure 5B shows an alignment of examples of protein kinases considered to have a phosphate binding pocket at the position equivalent to the said phosphate binding pocket of PDK1. Sequence conservation/preferred residues at the positions identified are discussed further in Example 1.

An amino acid sequence may be identifiable as that of a protein kinase catalytic domain by reference to sequence identity or similarities of three

dimensional structure with known protein kinase domains, as known to those skilled in the art.

Protein kinases show a conserved catalytic core, as reviewed in Johnson et al (1996) Cell, 85, 149-158 and Taylor & Radzio-Andzelm (1994) Structure 2, 345-355. This core folds into a small N-terminal lobe largely comprising anti-parallel β -sheet, and a large C-terminal lobe which is mostly α -helical. A deep cleft at the interface between these lobes is the site of ATP binding, with the phosphate groups near the opening of the cleft.

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Protein kinases also show conserved sequences within this catalytic core, and the residue equivalent to a given residue of, for example, PDK1, may be identified by alignment of the sequence of the kinase with that of known kinases in such a way as to maximise the match between the sequences. The alignment may be carried out by visual inspection and/or by the use of suitable computer programs, for example the GAP program of the University of Wisconsin Genetic Computing Group, which will also allow the percent identity of the polypeptides to be calculated. The Align program (Pearson (1994) in: Methods in Molecular Biology, Computer Analysis of Sequence Data, Part II (Griffin, AM and Griffin, HG eds) pp 365-389, Humana Press, Clifton).

The comparison of amino acid sequences or three dimension structure (for example from crystallography or computer modelling based on a known structure) may be carried out using methods well known to the skilled man, for example as described in WO 01/44497.

MAP kinase, MEK1, Cdk2 and Erk2 (for example) are not protein kinases having a hydrophobic pocket in the position equivalent to the hydrophobic (PIF binding) pocket of PDK1. MEK1, Cdk2 and ERK2 may have a larger

hydrophobic pocket which interacts with an amino acid sequence motif (which may be Phe-Xaa-Phe-Pro) which is not Phe-Xaa-Xaa-Phe. Thus, these protein kinases do not have a hydrophobic pocket in the position equivalent to the said hydrophobic (PIF-binding) pocket of PDK1.

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A further aspect of the invention provides a mutated protein kinase, wherein the protein kinase before mutation has a hydrophobic pocket in the position equivalent to the hydrophobic pocket (PIF-binding pocket) of human PDK1 that is defined by residues including Lys115, Ile118, Ile119, Val124, Vall27 and/or Leu155 of full-length human PDK1 and further has a phosphate binding pocket in the position equivalent to the phosphate binding pocket of human PDK1 that is defined by residues including Lys76, Arg131, Thr148 and/or Gln150, and wherein one or more residues equivalent to Ile118, Val124, Val127, Lys76 or Thr148 forming part of the hydrophobic pocket or phosphate binding pocket of the protein kinase is mutated. It is preferred that the said protein kinase is PDK1. The said protein kinase may alternatively be, for example, SGK, PKB or p70 S6 kinase. It is particularly preferred that the residue at the position equivalent to residue Lys76 of PDK1 is mutated to an Ala. The mutated protein kinase may be useful in determining whether a polypeptide or compound interacts with the hydrophobic (PIF binding) pocket or phosphate binding pocket of the unmutated protein kinase. For example, the abilities of a compound (including polypeptide) to bind to the mutated and unmutated protein kinase, or to modulate the activity of the protein kinase towards one or more substrates of the protein kinase, may be measured and compared.

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A further aspect of the invention provides a polynucleotide encoding a mutated protein kinase of the invention. A still further aspect of the invention provides a recombinant polynucleotide suitable for expressing a

mutated protein kinase of the invention. A yet further aspect of the invention provides a host cell comprising a polynucleotide of the invention.

A further aspect of the invention provides a method of making a mutated protein kinase of the invention, the method comprising culturing a host cell of the invention which expresses said mutated protein kinase and isolating said mutated protein kinase.

A further aspect of the invention provides a mutated protein kinase obtainable by the above method.

Examples of these aspects of the invention are provided in Example 1, and may be prepared using routine methods by those skilled in the art, for example as described in WO 00/35946.

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For example, the above mutated protein kinase may be made by methods well known in the art and as described below and in Example 1 or 2, for example using molecular biology methods or automated chemical peptide synthesis methods.

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It will be appreciated that peptidomimetic compounds may also be useful. Thus, by "polypeptide" or "peptide" we include not only molecules in which amino acid residues are joined by peptide (-CO-NH-) linkages but also molecules in which the peptide bond is reversed. Such retro-inverso peptidomimetics may be made using methods known in the art, for example such as those described in Mézière et al (1997) J. Immunol. 159, 3230-3237, incorporated herein by reference. This approach involves making pseudopeptides containing changes involving the backbone, and not the orientation of side chains. Retro-inverse peptides, which contain NH-CO

bonds instead of CO-NH peptide bonds, are much more resistant to proteolysis.

Similarly, the peptide bond may be dispensed with altogether provided that an appropriate linker moiety which retains the spacing between the $C\alpha$ atoms of the amino acid residues is used; it is particularly preferred if the linker moiety has substantially the same charge distribution and substantially the same planarity as a peptide bond.

It will be appreciated that the peptide may conveniently be blocked at its Nor C-terminus so as to help reduce susceptibility to exoproteolytic digestion.

The invention further provides a method of identifying a compound that modulates the protein kinase activity of a protein kinase having a hydrophobic pocket and phosphate binding pocket in the positions equivalent to the hydrophobic (PIF binding) pocket and phosphate binding pocket of PDK1, as defined above (for example PDK1), comprising the step of determining the effect of the compound on the protein kinase activity of, or ability of the compound to bind to the said mutated protein kinase of the invention.

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The method may further comprise determining the effect of the compound on the protein kinase activity of, or ability of the compound to bind to, the protein kinase (for example PDK1) which is not mutated at the said residue. When the protein kinase is PDK1, it may lack a functional PH domain (ie it may lack a PH domain capable of binding a phosphoinositide).

It will be appreciated that the protein kinase or mutated protein kinase may be a fusion protein comprising a tag, for example to aid purification, for example a GST tag, as described in Example 1.

The capability of the said PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase) polypeptide with regard to interacting with or binding to a polypeptide or other compound may be measured by any method of detecting/measuring a protein/protein interaction or other compound/protein interaction, as discussed further below. Suitable methods include methods analagous to those described in Example 1, as well as other methods, for example yeast two-hybrid interactions, co-purification, ELISA, co-immunoprecipitation and surface plasmon resonance methods. Thus, the said PDK1 (or SGK, PKB, PKA or p70 S6 kinase) may be considered capable of binding to or interacting with a polypeptide or other compound if an interaction may be detected between the said PDK1 polypeptide and the said interacting polypeptide by ELISA, co-immunoprecipitation or surface plasmon resonance methods or by a yeast two-hybrid interaction or copurification method, for example as described in Example 1.

It is preferred that the interaction can be detected using a surface plasmon resonance method, as described in Example 1. The interacting polypeptide (for example a polypeptide comprising a phosphorylated "hydrophobic motif", for example S6K-pHM; see example 1) may be immobilised on the test surface, for example it can be coupled through amino groups to a SensorChip CM5TM, according to the manufacturer's instructions, or a biotinylated polypeptide can be bound to an avidin coated SensorChip SA. The protein kinase (at concentrations between, for example 0 and between 10μM and 1.0μM, for example 2μM) is then injected over the surface and steady state binding determined in each case. From these measurements a K_d can be determined. It is preferred that the interaction has a K_d of less than 8μM, more preferably less than 5μM, 2μM, 1μM, 500nM, 300nM, 200nM or 100nM, for example about 150nM. Alternatively, a K_d can be determined for a polypeptide or other compound in competition with the immobilised polypeptide (or other compound). The protein kinase (for

example at a concentration of 0.5 µM) is mixed with free polypeptide (for example, at concentrations between 0 and 3 µM) and the mixture injected over the immobilised polypeptides. The steady state binding is determined in each case, from which the K_d of the interaction can be determined using the Cheng-Prescott relationship. Alternatively, the interaction may be expressed in terms of an observed response or relative observed responses, measured in terms of mass of protein bound to the surface, as described in Example 2. For example, the polypeptide may be immobilised by amino coupling to a SensorChip CM5 and each protein kinase (for example different mutated protein kinases, as discussed below) for example at a concentration of 1.0 µM or a range of concentrations, injected over the immobilised polypeptide. Alternatively, the polypeptide may be immobilised on a SA SensorChip and each protein kinase, for example at a concentration of 40nM or a range of concentrations injected over the immobilised polypeptide. The steady state response for each protein kinase is determined, for example expressed in Response Units (RU). 1000RU corresponds to 1 ng/mm² of protein bound to the surface. A response of less than 10RU may indicate that no interaction has taken place. A response of at least 10RU may indicate that the immobilised and injected molecules interact with each other.

It will be appreciated that the above methods may be used to determine whether a particular polypeptide or compound interacts with a protein kinase or mutated protein kinase.

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The effect of the compound on the rate or degree of phosphorylation of a hydrophobic pocket and/or phosphate binding pocket-dependent substrate may be determined. A compound may be selected that decreases the protein kinase activity of the said protein kinase, for example PDK1, towards a hydrophobic pocket-dependent substrate or a phosphate binding

pocket-dependent substrate and does not affect or increases the protein kinase activity towards a hydrophobic pocket or phosphate binding pocket-independent substrate, for example PKB when the kinase is PDK1. An activator of PDK1 may mimic insulin and may be useful in treating diabetes or obesity, and may protect cells from apoptosis.

Compounds that bind specifically to the phosphate binding site may activate PDK1 (or other AGK kinase having a phosphate binding site). Also compounds that bind to the residues forming part of the pohsphate binding site might transduce the negative effect and inhibit the kinase activity. A compound interacting with the phosphate binding site of PDK1 may be an activator, but only of a subset of substrates. Some substrates of PDK1 require the interaction with the phosphate binding site, such as S6K and SGK.

To generate a specific molecule that could bind to the phosphate and/or PIF-binding pocket of PDK1 a anti-idiotype strategy using combinatorial RNA libraries could be employed. Previous studies have established that Combinatorial RNA libraries can be used to isolate specific ligands, called aptamers, for virtually any target molecule by a procedure probably best known as SELEX (Ellington, A. D., and Szostak, J. W. (1990) Nature 346, 818-822; Tuerk, C., and Gold, L. (1990) Science 249, 505-510). Using this approach RNA molecules that interact with antibodies raised against PIFtide or peptides that encompass the hydrophobic motif of AGC kinases which are phosphorylated at their hydrophobic motif would be selected (preferably antibodies that are specific for the phosphorylated form ie bind the phosphorylated form but not the non-phosphorylated form). These RNA species then may have the intrinsic conformation to interact with the phosphate binding (and possibly also the PIF-binding) pocket(s) of PDK1.

Antibodies to the phosphate binding pocket may be produced. For example, animals could be immunised with wild type PDK1. Serum could then be purified with a column where the resin is coated with wild type PDK1 used for the immunisation. Specific antibodies could then be passed through columns coated with mutant PDK1 molecules differing only in that they have specific mutations in the phosphate binding pocket, such as Arg131, Lys76 or Gln150, for example mutated to Ala. Antibodies that don't bind to this mutant will either be specific antibodies that recognise the specific motifs or antibodies that are sensitive to the conformational changes associated with these mutations. The opposite development could also be performed: antibodies against a mutant PDK1 having a specific mutation(s) in the phosphate binding pocket, such as Arg131, Lys76 or Gln150, for example mutated to Ala, could be produced and the serum further purified through columns coated with wild type PDK1.

Thus, a further aspect of the invention provides an antibody reactive with the phosphate binding pocket of PDK1 or other hydrophobic pocket (PIF binding pocket)-containing protein kinase having a hydrophobic pocket in the position equivalent to the hydrophobic pocket of human PDK1 that is defined by residues including Lys115, Ile118, Ile119, Val124, Val127 and/or Leu155 of full-length human PDK1 and further having a phosphate binding pocket in the position equivalent to the phosphate binding pocket of human PDK1 that is defined by residues including Lys76, Arg131, Thr148 and/or Gln150. A further aspect of the invention provides an antibody reactive with PDK1 or other phosphate-binding pocket—containing protein kinase as defined above but not with the said protein kinase mutated at the phosphate binding site, or *vice versa*. A further aspect of the invention provides a method for preparing or selecting an antibody wherein the antibody is prepared or selected against a said protein kinase (for example

PDK1) unmutated at the phosphate binding site and a said protein kinase mutated at the phosphate binding site.

By the term "antibody" is included synthetic antibodies and fragments and variants (for example as discussed above) of whole antibodies which retain the antigen binding site. The antibody may be a monoclonal antibody, but may also be a polyclonal antibody preparation, a part or parts thereof (for example an F_{ab} fragment or $F(ab')_2$) or a synthetic antibody or part thereof. Fab, Fv, ScFv and dAb antibody fragments can all be expressed in and secreted from *E. coli*, thus allowing the facile production of large amounts of the said fragments. By "ScFv molecules" is meant molecules wherein the V_H and V_L partner domains are linked via a flexible oligopeptide. IgG class antibodies are preferred.

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Suitable monoclonal antibodies to selected antigens may be prepared by known techniques, for example those disclosed in "Monoclonal Antibodies: A manual of techniques", H. Zola (CRC Press, 1988) and in "Monoclonal Hybridoma Antibodies: techniques and Applications", JGR Hurrell (CRC Press, 1982), modified as indicated above. Bispecific antibodies may be prepared by cell fusion, by reassociation of monovalent fragments or by chemical cross-linking of whole antibodies. Methods for preparing bispecific antibodies are disclosed in Corvalen et al, (1987) Cancer Immunol. Immunother. 24, 127-132 and 133-137 and 138-143.

A general review of the techniques involved in the synthesis of antibody fragments which retain their specific binding sites is to be found in Winter & Milstein (1991) *Nature* 349, 293-299.

For example, an antibody that does not bind PDK1 Arg131Ala could be specifically recognising this residue in the phosphate binding site, but could

also be recognising specifically the inactive conformation of PDK1, which is stabilised by Arg 131. The opposite development could also be performed: antibodies against a mutant PDK1 Arg131Ala could be produced and the serum further purified through columns coated with wild type PDK1. In this way, antibodies may be prepared that would either not be able to interact with the phosphate binding site Arg 131 but only when a small residue is in its place, or antibodies that are probes for the active conformation of PDK1. These conformational probes could be used in high throughoutput screenings, HTS, in the search of compounds that are capable of modifying the conformation of the given protein kinase. Antibodies could have been produced with previous knowledge to detect active protein kinases by immunising with active protein kinases, but in those cases, the antibodies would have recognised also the phosphorylation events that make a protein kinase be active. In the methodology here described using the conformational probes could be easily isolated. antibodies. Furthermore, antibodies obtained from an active protein kinase (with overall modifications that make it active) could be further purified through a column coated with the inactive protein kinase (keeping the non bound fraction) and then further purifyied on a column coated with a protein kinase consisting of an activating mutation (such as R131A in the case of PDK1), retaining the specifically bound fraction, which could be an active conformation probe. This type of approach could also allow the development of conformation specific probes by the use of activating or inhibiting mutations.

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A further aspect of the invention provides a kit of parts useful in carrying out a method according to the preceding aspect of the invention, comprising (1) a mutated protein kinase of the invention and (2) the protein kinase which is not a mutated said protein kinase as defined above.

The protein structures described herein (for example with the co-ordinates shown in Examples 2, 3 or 4, or structures modelled thereon) may be useful in designing further reagents that may be useful in drug screening assays or characterisation of protein kinase activity or regulation. For example, such structures may be useful in designing mutants that may be useful in FRETbased activities, for example in which surface residues near to binding sites are mutated to cysteines to allow coupling of chromophores. For example, the cysteine residue may be fluorescently-labelled, and a change in fluorescence intensity or frequency may be detected in an assay. Any thiolreactive fluorophore, for example BADAN (see, for example, Wadum et al Fluorescently labeled bovine acyl-CoA binding protein - an acyl-CoA sensor. Interaction with CoA and acyl-CoA esters and its use in measuring free acyl CoA esters and non-esterified fatty acids (NEFA); Hammarstrom et al (2001) Biophys J 80(6), 2867-2885; Schindel et al (2001) Eur J Biochem 268(3), 800-808), could be used to label the cysteine. An alternative suitable fluorophore is Acrylodan (Richieri et al (1992) J Biol Chem 267(33), 23495-23501).

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20 It will be appreciated that the invention provides screening assays for drugs which may be useful in modulating, for example either enhancing or inhibiting, the protein kinase activity of a protein kinase (for example, the protein kinase activity towards a particular substrate) having a hydrophobic pocket in the position equivalent to the hydrophobic pocket of Protein Kinase A (PKA) that is defined by residues including Lys76, Leu116, Val80 and/or Lys111 of full-length mouse PKA, for example PDK1, SGK, PKB, PKA or p70 S6 kinase, for example the PDK1 or PDK2 activity (as discussed above) of PDK1. The compounds identified in the methods may

themselves be useful as a drug or they may represent lead compounds for the design and synthesis of more efficacious compounds.

The compound may be a drug-like compound or lead compound for the development of a drug-like compound for each of the above methods of identifying a compound. It will be appreciated that the said methods may be useful as screening assays in the development of pharmaceutical compounds or drugs, as well known to those skilled in the art.

The term "drug-like compound" is well known to those skilled in the art, and may include the meaning of a compound that has characteristics that may make it suitable for use in medicine, for example as the active ingredient in a medicament. Thus, for example, a drug-like compound may be a molecule that may be synthesised by the techniques of organic chemistry, less preferably by techniques of molecular biology or biochemistry, and is preferably a small molecule, which may be of less than 5000 daltons. A drug-like compound may additionally exhibit features of selective interaction with a particular protein or proteins and be bioavailable and/or able to penetrate cellular membranes, but it will be appreciated that these features are not essential.

The term "lead compound" is similarly well known to those skilled in the art, and may include the meaning that the compound, whilst not itself suitable for use as a drug (for example because it is only weakly potent against its intended target, non-selective in its action, unstable, difficult to synthesise or has poor bioavailability) may provide a starting-point for the design of other compounds that may have more desirable characteristics.

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It is appreciated that screening assays which are capable of high throughput operation are particularly preferred. Examples may include cell based

assays and protein-protein binding assays. An SPA-based (Scintillation Proximity Assay; Amersham International) system may be used. For example, beads comprising scintillant and a substrate polypeptide or interacting polypeptide may be prepared. The beads may be mixed with a sample comprising ³²P- or ³³P-γ-labelled PDK1 or other protein kinase or mutated protein kinase (as defined above) and with the test compound. Conveniently this is done in a 96-well or 384-well format. The plate is then counted using a suitable scintillation counter, using known parameters for ³²P or ³³P SPA assays. Only ³²P or ³³P that is in proximity to the scintillant, i.e. only that bound to the substrate or interacting polypeptide that is bound to the beads, is detected. Variants of such an assay, for example in which the substrate or interacting polypeptide is immobilised on the scintillant beads *via* binding to an antibody or antibody fragment, may also be used.

It will be understood that it will be desirable to identify compounds that may modulate the activity of the protein kinase in vivo. Thus it will be understood that reagents and conditions used in the method may be chosen such that the interactions between, for example, the said protein kinase and the interacting polypeptide, are substantially the same as between the human protein kinase and a naturally occurring interacting polypeptide comprising the said amino acid sequence. It will be appreciated that the compound may bind to the protein kinase, or may bind to the interacting polypeptide.

The compounds that are tested in the screening methods of the assay or in other assays in which the ability of a compound to modulate the protein kinase activity of a protein kinase, for example a hydrophobic pocket-containing protein kinase, as defined above, may be measured, may be compounds that have been selected and/or designed (including modified)

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using molecular modelling techniques, for example using computer techniques.

A further aspect of the invention is a compound identified or identifiable by the above selection/design methods of the invention, for example an RNA molecule or antibody identifiable as defined above.

A still further aspect of the invention is a compound (or polypeptide or polynucleotide) of the invention or identified or identifiable by the above selection/design methods of the invention, for use in medicine. Conditions or diseases in which such compounds, polypeptides or polynucleotides may be useful are indicated below.

The compound (or polypeptide or polynucleotide) may be administered in any suitable way, usually parenterally, for example intravenously, intraperitoneally or intravesically, in standard sterile, non-pyrogenic formulations of diluents and carriers. The compound (or polypeptide or polynucleotide) may also be administered topically, which may be of particular benefit for treatment of surface wounds. The compound (or polypeptide or polynucleotide) may also be administered in a localised manner, for example by injection. The compound may be useful as an antifungal (or other parasitic, pathogenic or potentially parasitic or pathogenic organism) agent.

A further aspect of the invention is the use of a compound (or polypeptide or polynucleotide) as defined above in the manufacture of a medicament for the treatment of a patient in need of modulation of signalling by a protein kinase having a hydrophobic/phosphate binding pocket, as defined above, for example PDK1, SGK, PKB or p70 S6 kinase, for example insulin signalling pathway and/or PDK1/PDK2/SGK/PKB/p70 S6

kinase/PRK2/PKC signalling. The patient may be in need of inhibition of a said hydrophobic/phosphate binding pocket-containing kinase in an infecting organism, for example the patient may have a fungal infection for which treatment is required. The compound may inhibit the infecting organism's (for example fungal) hydrophobic/phosphate binding pocket-containing protein kinase, but may not inhibit the patient's equivalent hydrophobic/phosphate binding pocket-containing protein kinase.

A further aspect of the invention is a method of treating a patient in need of modulation of signalling by a protein kinase having a hydrophobic/phosphate binding pocket as defined above, for example PDK1, SGK, PKB or p70 S6 kinase, for example insulin signalling pathway and/or PDK1/PDK2/SGK/PKB/p70 S6 kinase/PRK2/PKC signalling, wherein the patient is administered an effective amount of a compound (or polypeptide or polynucleotide) as defined above.

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A compound that is capable of reducing the activity of PKC, for example PKCβ, PRK1 or 2, PDK1 (ie the PDK1 and/or the PDK2 activity), PKB, SGK or p70 S6 kinase may be useful in treating cancer. PDK1, for example via PKB and/or SGK, may be capable of providing a survival signal that protects cells from apoptosis induced in a variety of ways (reviewed in Cross et al (1995) Nature 378, 785-789 and Alessi & Cohen (1998) Curr. Opin. Genetics. Develop. 8, 55-62). Thus, such compounds may aid apoptosis. Reduction of the activity of PDK1, PKB, SGK and/or p70 S6 kinase may promote apoptosis and may therefore be useful in treating cancer. Conditions in which aiding apoptosis may be of benefit may also include resolution of inflammation.

A compound is capable of increasing the activity of PDK1, PKB, SGK or p70 S6 kinase may be useful in treating diabetes or obesity, or may be

useful in inhibiting apoptosis. Increased activity of PDK1, PKB, SGK or p70 S6 kinase may lead to increased levels of leptin, as discussed above, which may lead to weight loss; thus such compounds may lead to weight loss. For example, such compounds may suppress apoptosis, which may aid cell survival during or following cell damaging processes. It is believed that such compounds are useful in treating disease in which apoptosis is involved. Examples of such diseases include, but are not limited to, mechanical (including heat) tissue injury or ischaemic disease, for example stroke and myocardial infarction, neural injury and myocardial infarction. Thus the patient in need of modulation of the activity of PDK1, PKB, SGK or p70 S6 kinase may be a patient with cancer or with diabetes, or a patient in need of inhibition of apoptosis, for example a patient suffering from tissue injury or ischaemic injury, including stroke.

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- Thus, a further aspect of the invention provides a method of treating a patient with an ischaemic disease the method comprising administering to the patient an effective amount of a compound identified or identifiable by the screening methods of the invention.
- A still further invention provides a use of a compound identifiable by the screening methods of the invention in the manufacture of a medicament for treating an ischaemic disease in a patient.
- Thus, a further aspect of the invention provides a method of treating a patient with an ischaemic disease the method comprising administering to the patient an effective amount of a compound identifiable by the screening methods of the invention.

If the patient is a patient in need of promotion of apoptosis, for example a patient with cancer, it is preferred that the compound of the invention that is

used in the preparation of the medicament is capable of reducing the activity of PDK1, PKB, SGK or p70 S6 kinase. If the patient is a patient with diabetes or a patient in need of inhibition of apoptosis, for example a patient with ischaemic disease, it is preferred that the compound of the invention that is used in the preparation of the medicament is capable of increasing the activity of PDK1, PKB, SGK or p70 S6 kinase.

All documents referred to herein are hereby incorporated by reference.

The invention is now described in more detail by reference to the following, non-limiting, Figures and Examples.

Figure legends

15 1. Overview of the PDK1 structure.

The PDK1 kinase domain backbone is shown in a ribbon representation, with the secondary structure elements for residues 74-163 in the lower half of the Figure and for residues 164- 358 in the upper part of the Figure. Helix αG , encompassing residues 287-295 (which makes a crystal contact to a symmetry related PDK1 molecule, Fig. 2), is at the bottom right of the Figure. Key residues discussed in the text are shown as a sticks model. ATP is shown as a sticks model. A simulated annealing $|Fo-|Fc\rangle$, ϕ calc map is shown in black, contoured at 3 σ . The phosphoserine and the sulphate discussed in the text are also shown.

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2. The PIF-pocket

A. A surface representation of the putative PIF binding pocket is shown and compared to the pocket interacting with the C-terminal FXXF motif in PKA. For PDK1, the αG helix of a symmetry-related molecule is shown as

a ribbon, in PKA the C-terminus is also shown as a ribbon. Aromatic amino acids buried in the pocket are shown as sticks; further side chains interacting with the pocket are also shown as sticks. Helix α C is also shown as a ribbon in both PDK1 and PKA (at bottom of images). In PDK1, the ordered sulphate ion and basic residues interacting with it are also shown.

B. A stereo image of the residues lining the PIF-pocket is shown. The PDK1 backbone is shown as a grey ribbon. Side chains are shown as sticks. Hydrogen bonds to the sulphate ion are shown as black dotted lines.

3. Structure-based sequence alignment

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The sequences of PKA and PDK1 are aligned according to a structural superposition performed in WHAT IF [Vriend, 1990]. Sequence numbering is according to PDK1. β -strands (arrows) and α -helices (bars) are shown for the PDK1 structure according to a DSSP [Kabsch and Sander, 1983] secondary structure assignment, and labelled consistent with the secondary structure element names proposed for PKA [Taylor and Radzioandzelm, 1994]. Residues lining the PIF-pocket are indicated with a black dot. Residues hydrogen bonding the sulphate ion are indicated by arrows. The PDK1 residues equivalent to Ser53 and Gly186 in PKA, are labelled with an asterisk.

4. PDK1 binding & activation studies

Binding and activation of wild type and mutant forms of PDK1 to a phosphopeptide derived from the hydrophobic motif of S6K1. The binding of the wild type (wt) PDK1 and indicated mutants to a phosphopeptide comprising the hydrophobic motif of S6K1 (S6K-pHM: SESANQVFLGFT*YVAPSV, where T* indicates phospho-threonine) was analysed by surface plasmon resonance as described in the Materials and Methods.

A. The sensor chip SA was coated with 12RUs of the biotinylated S6K-pHM peptide and the binding was analysed following injection of 270 nM wild type PDK1, PDK1 [T148A] and PDK1 [K76A]. No detectable binding to S6K-pHM was observed using PDK1 [R131A] or PDK1 [Q150] (data not shown).

B. As in A. except that binding was analysed over a range of PDK1 concentrations (2-2150nM). The response level at the steady state binding is plotted versus the log of the PDK1 concentration. The estimated Kd was obtained by fitting the data to a sigmoid curve using Kaleidagraph software.

10 Kd for wild type PDK1 was 642 - 131 nM, PDK1 [T148A] was 64 - 7 nM and PDK1 [K76A] was 1744 - 167 nM. No detectable binding of PDK1 to the non-phosphorylated S6K-HM peptide (SESANQVFLGFTYVAPSV) was detected with wild type PDK1 or any of the mutants (data not shown).

C. Activation of the indicated forms of PDK1 by S6K-pHM and S6K-HM. PDK1 activity was measured using the peptide substrate (T308tide) in the presence of the indicated concentrations of S6K-pHM (closed circles) and S6K-HM (open circles) as described in the methods. Assays were performed in triplicate and similar results obtained in 2 separate experiments. The results are the average – SD for a single experiment.

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5. Interactions of regulatory phosphates with the αC helix

A. The PDK1 backbone is shown as a ribbon, with helix α C in the centre of the view. Key residues are shown as sticks. The sulphate ion and the phosphate on the activation loop are also shown. A sticks model of ATP is shown. Hydrogen bonds are shown as black dotted lines.

B. Alignment of the amino acid sequence forming part of the phosphate pocket on PDK1 with the equivalent region of the indicated AGC kinases. Identical residues are denoted by white letters on a black background and similar residues by gray boxes. Arrows indicate the residues corresponding

30 to Lys 76, Arg131, Thr148 and Gln150 of PDK1.

6. Essential dynamics

- A. Projection of all available PKA crystal structures (labelled dots) and the PDK1 structure (diamond) onto the first two eigenvectors (i.e. the ones with the two largest eigenvalues) calculated from the PKA structures.
- B. Graphic representation of the motion along the first eigenvector, generated by projecting two structures at -4 nm (black) and +4 nm (grey).

7. Alignment of AGC protein kinase family members.

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Example 1: High resolution crystal structure of the human PDK1 catalytic domain defines the regulatory phosphopeptide docking site

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The 3-Phosphoinositide Dependent Protein Kinase-1 (PDK1) plays a key role in insulin/growth factor induced signalling pathways through phosphorylation of downstream AGC-kinases such as Protein Kinase B/Akt and p70 ribosomal S6 kinase (S6K1). Here we describe the 2.0 Å crystal structure of the PDK1 kinase domain in complex with ATP. The structure defines the hydrophobic pocket termed the 'PIF-pocket'which plays a key role in mediating the interaction and phosphorylation of certain substrates such as S6K1. In the PDK1 structure, this pocket is occupied by an extensive crystallographic contact with another molecule of PDK1, reminiscent of the interaction of Protein Kinase A with the hydrophobic motif at its C-terminus. Previous studies have shown that phosphorylation of S6K1 at its C-terminal PIF-pocket-interacting motif, promotes the binding of S6K1 with PDK1, suggesting that there may be a phosphate docking site located nearby the PIF-pocket. Interestingly, close to the PIF-pocket on the PDK1 structure, there is an ordered sulphate ion, interacting

tightly with four surrounding side chains. The roles of these residues were investigated through a combination of site directed mutagenesis and kinetic studies, the results of which suggest that this region of PDK1 does indeed represent a phosphate dependent docking site. An analogous phosphate binding regulatory motif may participate in the activation of other AGC kinases.

Results & Discussion

Overall structure

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The structure of the catalytic domain of PDK1 was solved by molecular replacement and refined to an R-factor of 0.19 (Rfree=0.22). PDK1 assumes the classic bilobal kinase fold (Fig. 1) and is similar to the only other AGC kinase structure solved, that of PKA (RMSD of 1.0 Å on C α atoms with PDB entry 1STC [Prade et al., 1997]). The form of PDK1 that was crystallized comprised residues 51 to 359. The tip of the activation loop (residues 233-236) is disordered, as observed in other kinase structures [Johnson et al., 1996]. The N-terminus (residue 51-70), which is pointing into a large void generated by the crystallographic symmetry, is also disordered. In contrast, the N-terminal extension to the kinase domain of PKA assumes an amphipathic a -helix (termed αA-helix), and packs against the kinase core [Knighton et al., 1991]. The cluster of hydrophobic residues that mediates this interaction in PKA is not present in PDK1, suggesting that the N-terminus of PDK1 could have a different function from that of PKA. Interestingly, it has recently been shown that the N-terminus of PDK1 (residues 1-50) interacts with Ral guanine nucleotide exchange factors [Tian et al., 2002]. Thus, this region may assume a unique conformation in PDK1, which is not defined by the structure described here.

PDK1 was crystallised in the presence of ATP but in the absence of any divalent cations. In the early stages of the refinement well-defined density for the entire ATP molecule could be observed. ATP adopts a different conformation to that observed in other kinase-ATP complexes (Fig. 1). Perhaps due to the absence of divalent cations, the generally observed kink between the β and γ phosphate caused by the interaction with such an ion, is not seen in the PDK1 structure.

It is known that PDK1 can phosphorylate itself on residue Ser 241 in the activation loop and that this phosphorylation is required for PDK1 activity [Alessi et al., 1997]. Indeed, we observed density for a phosphate attached to this residue (Fig. 1), and extensive interactions are observed between this phosphoserine and residues from the C-terminal lobe and α C-helix (Fig. 1). The interaction between Ser241 and the C-terminal lobe is similar to the equivalent interactions in PKA but as discussed below the binding to the α C-helix differs.

The PIF-pocket

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As outlined in the introduction, PDK1 was postulated to possess a pocket (the 'PIF-pocket') in the small lobe of its catalytic domain, required for the binding of PDK1 to the hydrophobic motif of its substrates [Biondi et al., 2000]. The PDK1 structure described here indeed reveals such a pocket, and shows that it lies in a location similar to the FXXF-binding pocket in PKA (Fig. 2). PDK1 residues Lys115, Ile118, Ile119 on the αB helix (Fig. 2), Val124, Val127 on the αC helix and Leu155 on β-sheet 5 form an approximately 5 Å deep pocket. Previous work has shown that mutation of Leu 155 to Glu abolishes the ability of PDK1 to interact with a peptide that encompasses the hydrophobic motif of PRK2 (PIFtide) [Biondi et al., 2000]

as well as with S6K1, SGK1, PKCζ and PRK2 [Balendran et al., 2000, Biondi et al., 2000]. In addition, mutation of Lys115, Ile119, Glu150, and Leu155 to alanine, reduced the affinity of PDK1 for PIFtide approximately 10-fold, but did not affect the ability to phosphorylate and activate S6K1 and SGK1 [Biondi et al., 2001]. These results are in agreement with the crystal structure of the PIF-pocket, since Leu155 is located at the center and the other residues line the wall of the pocket (Fig. 2). Interestingly, in our structure, the PIF-pocket is occupied by helix αG of a symmetry related molecule (Fig. 2). Tyr288 and Phe291 make hydrophobic contacts in this pocket with almost all pocket-lining residues, remarkably reminiscent of the interactions of the phenylalanines in the FXXF motif in PKA and their hydrophobic docking site in the equivalent region of the kinase domain (Fig. 2). In addition, residues Glu287, Gln292, Ile295 and Lys296 on the symmetry related loop also form contacts with residues lining the PIFpocket. In total, 244 ² Å of accessible surface is buried by this contact, suggesting this is a tight interaction. However, the significance of this interaction is not clear as an oligomerisation event for PDK1 has not been demonstrated in solution previously. Indeed both the isolated catalytic domain of PDK1 that was crystallised and full length PDK1 migrate in gel filtration chromatography as apparent monomeric species (data not shown).

The phosphate pocket

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As outlined in the introduction, substrates of PDK1, such as S6K1, interact with the PIF-pocket of PDK1 with higher affinity when they are phosphorylated at their hydrophobic motif. This suggested that a regulatory phosphate binding site may be located close to the PIF-pocket. During refinement of the PDK1 structure, it became clear that next to the PIF-pocket another small pocket was present, occupied by a tetrahedral oxy-

anion (Fig. 2). As 2.0 M of sulphate was present in the crystallisation conditions, this was assigned as a sulphate ion. The ion interacts with four residues lining the pocket, namely Lys76, Arg131, Thr148 and Gln150. Because of its close proximity to the PIF-pocket (approximately 5Å) it is possible that this sulphate-occupied pocket could represent the binding site for the phosphate on the phosphopeptide. To investigate this further, we mutated Lys76, Arg131, Thr148 and Gln150 to Ala, in order to verify the contribution of each of these residues in enabling PDK1 to interact with a peptide encompassing the hydrophobic motif of S6K1, in which the residue equivalent to Thr412 was phosphorylated (termed S6K-pHM). A quantitative surface plasmon resonance based binding assay (Fig. 4A) showed that wild type PDK1 interacted with S6K-pHM, with a Kd of 0.6 μM with S6K-pHM but not detectably to the non-phosphorylated form of this peptide (S6K-HM). The PDK1[R131A] and PDK1[Q150A] mutants did not detectably interact with S6K-pHM in this assay (Fig. 4B), confirming that the interactions these residues make in the PDK1 structure are of key importance. The PDK1[K76A] mutant interacted with 3-fold lower affinity (Kd 1.7 μ M) with S6K-pHM. The PDK1[T148A] mutant however possessed about 10-fold higher (Kd 0.06 µM) affinity for S6KpHM than wild type PDK1. Moreover, the dissociation of PDK1[T148A] from S6K-pHM is markedly slower than that of wild type PDK1 or PDK1[K76A] (Fig 4A). These findings are unexpected as Thr148 is within hydrogen bonding distance of the sulphate (Fig. 2), but indicate that this residue may play a role in enabling the dissociation of PDK1 from S6KpHM.

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The binding of PDK1 to PIFtide stimulates up to 4-fold the rate at which PDK1 phosphorylates a small peptide that encompasses the activation loop motif of PKB (termed T308tide) [Biondi et al., 2000], indicating that occupancy of the PIF-pocket of PDK1 activates the enzyme. Similarly, the

binding of a phosphopeptide corresponding to the hydrophobic motif of RSK stimulated PDK1 activity 6-fold [Frodin et al., 2000]. We have now also found that the binding of S6K-pHM to wild type PDK1 induces a maximal 5-fold activation, with a half maximal activation occurring at a concentration of approximately 50 μM S6K-pHM (Fig. 4C). We next specific activities of PDK1[K76A], assayed the PDK1[R131A], PDK1[T148A] and PDK1[Q150A] mutants in the absence and presence of increasing concentrations of S6K-pHM (Fig. 4C). The PDK1[K76A] possessed the same specific activity towards T308tide in the absence of S6K-pHM as wild type PDK1, but an approximately 3-fold higher concentration of S6K-pHM was required to half maximally activate PDK1[K76A], consistent with the reduced affinity of this form of PDK1 for S6K-pHM (Fig. 4A,B). The PDK1[R131A] mutant possessed a 3-fold higher specific activity towards Thr308tide in the absence of S6K-pHM (Fig. 4C), as has been observed previously with certain other PIF-pocket mutants of PDK1(PDK1[K115A] and PDK1[L155E]) [Biondi et al., 2000]. However, in accordance with the inability of PDK1[R131A] to bind S6KpHM in the Biacore assay (Fig. 4B), it was not significantly activated by concentrations of S6K-pHM below 0.1 mM and its activity was only moderately further increased by the addition of high concentrations (0.3 and 1 mM) of S6K-pHM (Fig. 4C). The activity of a mutant of PDK1 in which both Lys76 and Arg131 were changed to Ala was activated even less significantly by these high concentrations of S6K-pHM. The PDK1[T148A] and PDK1[Q150A] mutants possessed similar specific activity towards T308tide as wild type PDK1 in the absence of S6K-pHM. The PDK1[T148A] mutant was activated similarly as wild type PDK1 by S6KpHM and consistent with the inability of PDK1[Q150A] to interact with S6K-pHM, this mutant of PDK1 was not significantly activated by concentrations of S6K-pHM below 0.1 mM but at 0.3 and 1 mM peptide a 2-3 fold activation was observed (Fig. 4).

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At very high peptide concentrations (0.3-1 mM) the non-phosphorylated S6K-HM peptide induced a small (<2-fold) activation of PDK1 (Fig. 4C). Interestingly, despite the PDK1[K76A] and PDK1[R131A] mutants being markedly less able to interact with the phosphorylated S6K-pHM peptide, than wild type PDK1, high concentrations of the S6K-HM peptide activated PDK1[K76A] and PDK1[R131A] to a similar extent as wild type PDK1, indicating that the ability of these mutants to interact weakly with the S6K-HM peptide was not affected.

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We evaluated the sequence conservation in the phosphate pocket of the insulin/growth factor-activated AGC family kinases (PKB α , S6K1, SGK1 and RSK1). Sequence alignments indicate that this pocket is conserved amongst these kinases (Fig 5A). The most conserved residue is Gln150 which is found in all of these AGC kinases and the residue equivalent to Lys76 is always a basic residue (Fig. 5A). Arg131 is conserved in S6K1, SGK1 and RSK1 but not in PKB α , or PKB β or PKB γ , where it is an Asn or Ser. Thr148 is conserved in PKB α and SGK1 but is an Ala in S6K1 and RSK1. Interestingly, we have found the Thr 148Ala mutation in PDK1 did not disrupt the phosphate pocket (Fig 4). As PKB α , S6K1, SGK1 and RSK1 require to be phosphorylated at their hydrophobic motif to be maximally activated, it is tempting to speculate that the C-terminal hydrophobic motifs of these enzymes, when phosphorylated, bind to their own PIF/phosphate pockets, thereby generating a network of interactions similar to that of PDK1. In support of this, PKB $\!\alpha$, S6K1, SGK1 and RSK1 also require phosphorylation of their activation loop at the position equivalent to Ser241 for activity. Consistent with PKA not possessing a phosphate pocket, Lys76 and Gln150 are not conserved in PKA (Fig. 3), and indeed such a pocket is not observed in the PKA structure (Fig. 2).

The αC helix

The PDK1 structure shows that, as in other protein kinases [Johnson et al., 2001, Husen and Kuriyan, 2002], the α C helix (residues 124-136) is a key signal integration motif in the kinase core. One turn of the PDK1 α C helix (residues 129-131, Figs. 3, 5) links together the N-terminal lobe, the C-terminal lobe and the active site. Arg129 points towards the activation loop and forms two hydrogen bonds with the phosphorylated Ser241, whereas Arg131 forms two hydrogen bonds with the sulphate in the phosphate pocket (Fig. 5). Glu130 coordinates Lys111 which forms a hydrogen bond with the α -phosphate of the bound ATP. This interaction is conserved in all protein kinases and shown to be crucial for activation [Johnson et al., 2001, Husen and Kuriyan, 2002]. An additional residue, His126, forms a third hydrogen bond with the phosphorylated Ser241. Val124 and Val127 on the α C helix are involved in formation of the PIF-pocket (Fig. 5).

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The αC helix provides a structural link between the putative phosphopeptide binding pocket and the phosphoserine in the activation loop. The fact that R131A has higher basal activity than wild type PDK1 may indicate that this residue plays tuning role in the PDK1 structure, not only participating in the activation of PDK1 in the presence of a phosphate ion, but also on keeping the equilibrium of the enzyme towards an inactive conformation in the absence of S6K-pHM. To our knowledge this is the first report of a kinase structure in which the αC helix is positioned by 2 regulatory phosphate binding sites on either side of the helix (Fig 5). This provides a possible sensor-mechanism for linking the phosphorylation-state of the activation loop and the phosphopeptide binding event in the PIF-pocket to PDK1 activity.

Activation state

All structures of PKA solved to date show a phosphorylated T-loop and are therefore assumed to be in an active state. In addition to the unphosphorylated versus phosphorylated states of PKA, there appear to be two main conformational states possible for the latter [Zheng et al., 1993, Johnson et al., 2001]. In the active, closed conformation, all residues are positioned to facilitate phosphoryl transfer. In contrast, the inactive, open conformation is seen in absence of a nucleotide, and differs from the closed conformation by conformational changes of the N-terminal and C-terminal domains with respect to each other. In addition, three 'intermediate' structures were described from PKA, having either adenosine (PDB entry 1BKX [Narayana et al., 1997]) or the inhibitors staurosporine (PDB entry 1STC [Prade et al., 1997]) and balanol (PDB entry 1BX6 [Narayana et al., 1999]) in the ATP-binding site. Taylor and colleagues have described a method to distinguish between the active and inactive conformations, based on three distances: His87-pThr197 (aC helix positioning), Ser53-Gly186 (opening of the glycine-rich loop) and Glu170-Tyr330 (C-terminal tail distance to active site) [Johnson et al., 2001]. In PDK1, only one of these distances, the opening state of the glycine rich loop, can be measured due to sequence conservation (Fig. 3). This distance is 12.4 Å, similar to a PKA intermediate conformation (this distance in PKA is 14.2Å for the open, 11.8 Å for intermediate and 10.0 Å for the closed conformation [Johnson et al., 2001]). To allow a more direct comparison of the PDK1 structure with the available PKA structures, we have analysed the conformational state of PDK1 in detail using a novel approach, which involves a principal component analysis (also called "essential dynamics" [Amadei et al.,1993]) of the crystallographic coordinates. In short, this involves the construction of a covariance matrix containing the correlations between atomic shifts (with respect to an average structure) in the ensemble of all available PKA crystal structures. Diagonalisation of this matrix gives eigenvector/eigenvalue sets which describe concerted shifts of atoms

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(eigenvectors) together with the corresponding mean square fluctuation of the structures (eigenvalues). This approach allows a condensed description of PKA conformational states using only a few degrees of freedom, as shown previously for a range of other proteins [van Aalten et al., 1997,van Aalten et al., 2000,deGroot et al., 1998]. Diagonalisation of a covariance matrix built from the backbone atoms of residues 37-196, 198-283 and 286-305 results in a set of eigenvectors that describe concerted motions of the PKA backbone. In Fig. 6A, all PKA structures are projected on a subspace spanned by the first two eigenvectors (i.e. those with the two largest eigenvalues). It appears that the PKA structures cluster in three main areas along the first eigenvector. On the left of the average structure (which by definition has a projection of 0.0 on all eigenvectors) are the structures that are known to be in the "open" conformation (Fig. 6A). Around the average structure lie the structures that have been shown to be in an "intermediate" conformation (complexes with the inhibitors staurosporine, balanol and adenosine). More to the right of the average structure are the PKA structures that are known to be in the "closed" conformation. Thus, we have captured the conformational state of PKA in a single variable, the translation along the first eigenvector. This is further clarified by investigation of the atomic shifts described by this eigenvector in Cartesian space (Fig. 6B). A hinge-bending motion is observed between the Nterminal and C-terminal lobes, opening and closing the active site. It is now possible directly to compare the PDK1 conformational state by projecting the structure (backbone atoms only) onto the PKA eigenvectors. Fig. 6A shows that the conformation of PDK1 is close to the PKA structures that are in an "intermediate" conformation, consistent with the other structural analyses described above.

Conclusions

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We have reported the structure of the PDK1 catalytic domain, which, although similar to PKA, has revealed important features that increase our understanding of the mechanism by which PDK1 is regulated. The structure, together with mutational analyses, defines a phosphopeptide binding pocket, consisting of a separate hydrophobic PIF-pocket and a phosphate binding site, which mediates the interaction of PDK1 with the phosphorylated hydrophobic motif of S6K. This is consistent with the previous hypothesis that phosphorylation of S6K and SGK [Biondi et al., 2001] as well as RSK [Frodin et al., 2000] at their FXXFS/T hydrophobic motif is the trigger for their interaction and phosphorylation by PDK1. In this mechanism the PIF-pocket would physiologically only interact with the Phe residues when the Ser/Thr residue is phosphorylated. Furthermore, as the phosphate pocket is conserved in other AGC kinases, the structural features and network of interaction of the phosphate pocket with the α Chelix on PDK1, could provide insight into the mode of activation of other AGC kinases.

Experimental Procedures

20 Materials

Mammalian and Insect cells culture reagents were from Life, Technologies. SensorChips SA were from BiaCore AB. Glutathione Sepharose, as well as pre-packed HiTrap Q HP and Hiload Superdex 200 prep grade columns were from Amersham Biosciences. Dialysis cassettes were from the Slide-A-Lyzer series (Pierce). Ni-NTA Agarose was from Qiagen. Disposable ultrafiltration devices (polyethersulfone membranes) were from Vivascience. Crystallisation research tools (primary screens, additive

screens and crystallisation plates) were from Hampton Research. Peptides were synthesised by Dr G. Blomberg (University of Bristol, UK).

General methods

Molecular biology techniques were performed using standard protocols. Site directed mutagenesis was performed using a QuickChange kit (Stratagene) following instructions provided by the manufacturer. DNA constructs used for transfection were purified from bacteria using Qiagen plasmid Mega kit according to the manufacturer's protocol, and their sequence verified. Human kidney embryonic 293 cells were cultured on 10 cm diameter dishes in Dulbecco's modified Eagle's medium containing 10% foetal bovine serum.

Buffers

Low Salt Buffer: 25mM Tris-HCl pH 7.5, 150 mM NaCl; High Salt Buffer: 25mM Tris-HCl pH 7.5, 500 mM NaCl. Lysis Buffer: 25mM Tris-HCl pH 7.5, 150 mM NaCl 0.07% β -mercaptoethanol, 1mM Benzamidine, and 20 µg/ml PMSF. Buffer A: 50 mM Tris-HCl pH 7.5, 1 mM EGTA, 1 mM EDTA, 1% (by mass) Triton-X 100, 1 mM sodium orthovanadate, 50 mM sodium fluoride, 5 mM sodium pyrophosphate, 0.27 M sucrose, 1 µM microcystin-LR, 0.1% (by vol) β -mercaptoethanol and "complete" proteinase inhibitor cocktail (one tablet per 50 ml, Roche). Buffer B: 50 mM Tris/HCl pH 7.5, 0.1 mM EGTA, 10 mM β -mercaptoethanol and 0.27 M sucrose.

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Expression, purification and characterisation of the kinase domain of PDK1

A cDNA encoding for human PDK1 amino acid residues 51-359 with a stop codon inserted at position 360, was amplified by PCR reaction using full length human PDK1 cDNA in the pCMV5 vector [Alessi et al., 1997] as a template a 5'primer, which incorporates a BamH1 restriction site, an initiating methionine, a hexahistidine tag.followed by a PreScission protease recognition sequence prior to the residue equivalent to Met51 of PDK1 (ggatcctataaatatggcacatcatcatcatcatctggaagttctgttccaggggcccatggacggcact gcagccgagcctcgg) and the 3' primer applied in this reaction was: 5'ggatcctcaggtgagcttcggaggcgtctgctggtg-3'. The resulting PCR product was ligated into pCR 2.1 TOPO vector (Invitrogen) and then subcloned as a BamH1-BamH1 fragment into pFastbac1 vector (Life Technologies) for baculovirus protein expression. The resulting construct was then used to generate recombinant baculovirus using the Bac-to-Bac system (Life Technologies) following the manufacturer's protocol. The resulting baculoviruses were used to infect Sf21 cells at 1.5 x 106/ml. The infected cells were harvested by centrifugation 72 hours post infection. Cell pellets corresponding to 7 l of culture were resuspended in 900 ml of Lysis Buffer and cells lysed in nitrogen cavitation chamber. Cell debris was then pelleted by centrifugation, the supernatant made 0.5 M NaCl by addition of 4M NaCl and then incubated with Ni-NTA-Agarose (10 ml resin) for one hour. The resin was then washed in 10 times with 40 ml of Lysis Buffer containing 0.5M NaCl and then placed in a disposable Econo-Pac column (BioRad), where the resin was further washed with 700 ml of high salt buffer and then with 100 ml of low salt buffer, both supplemented with 10 mM imidazole. Elution was performed with 200 mM imidazole in high salt buffer and 2 ml fractions were collected. Fractions containing protein were. pooled, diluted to 200 mM NaCl with 25 mM Tris/HCl pH 7.5, and loaded onto a 5 ml Hi-trap Q sepharose column. The flow-through from this step, containing PDK1, was concentrated to 4 ml and then chromatographed on a 16/60 Superdex 200 gel filtration column using an AKTA Explorer system

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(Amersham Biosciences) equilibrated with high salt buffer with the addition of 1mM DTT. PDK1 eluted in a large symmetric peak at the expected size for a monomer. The PDK1 containing peak was again pooled, concentrated and incubated with 300 µg GST-PreScission protease (expression construct kindly provided by John Heath, University of Birmingham, UK) on ice for 4h. In order to eliminate the cleaved His-tag sequences as well as any remaining uncleaved His-PDK1 and the GST-PreScission protease, the mixture was incubated with a mixture of 200 µl glutathione-Sepharose and 200 µl Ni-NTA agarose resin for 15 minutes and the PDK1 protein that did not bind was collected. The resulting protein consists of PDK1 (51-359) preceded by a Gly-Pro at the N-terminus. The protein at this stage of the purification was apparently homogeneous as revealed by a single band after electrophoresis of 20 µg of protein on SDS-PAGE and staining with Coomasie Brilliant Blue R250 (data not shown).

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Electrospray mass spectrometry revealed a main peak mass close to the expected size of this fragment of PDK1. The specific activity of PDK1 (51-359) towards the peptide T308tide and its activation in the presence of PIFtide was identical to wild type full length PDK1 [Biondi et al., 2000], and tryptic peptide mass finger printing indicated that PDK1 was quantitatively phosphorylated at Ser241 (data not shown). In BiaCore experiments, the steady state binding of PDK1 (51-359) to the peptide PIFtide was similar to that of the His-tag PDK1 (51-556) protein characterised previously [Balendran et al., 1999a].

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Crystallisation and data collection

The PDK1 (51-359) protein was concentrated to a final concentration of 8.5 mg/ml (as determined by a Bradford assay using bovine serum albumin as a

standard). The sitting drop vapour diffusion method was used for producing crystals. Sitting drops were formed by mixing 1 µl of protein solution with 1 µl of a mother liquor solution (0.1 M Tris/HCl pH 8.5, 2.0 M ammonium sulphate, 16.6 mM ATP) with the addition of 0.2 µl EDTA (100mM). Hexagonal crystals (Table I) of PDK1 were grown at 20° C from a mother liquor containing 0.1M Tris/HCl pH 8.5, 2.0 M ammonium sulphate, 16.6 mM ATP). Crystals appeared after one day, growing to 0.05 x 0.05 x 0.2 mm over 20 days. Crystals were frozen in a nitrogen gas stream after being soaked in 0.075 M Tris 8.5, 1.5M ammonium sulphate, 25% (v/v) glycerol.

Expression and purification of wild type and mutant forms of GST-PDK1.

Wild type-PDK1 [Alessi et al., 1997], PDK1[R76A], PDK1[R131A], PDK1[R76A,R131A], PDK1[T148A] and PDK1[Q150A] in the pEBG2T vector were used to express the wild type and indicated mutants of PDK1 fused through their N-terminus to glutathione S-transferase (GST). The GST fusion proteins were expressed in human embryonic kidney 293 cells. For the expression of each construct, twenty 10 cm diameter dishes of 293 cells were cultured and each dish transfected with 10 µg of the pEBG-2T construct, using a modified calcium phosphate method. 36 h post-transfection, the cells were lysed in 0.6 ml of ice-cold Buffer A, the lysates pooled, centrifuged at 4 ° C for 10 min at 13000 g and the GST-fusion proteins were purified by affinity chromatography on glutathione-Sepharose and eluted in Buffer B supplemented with 20 mM glutathione as described previously [Alessi et al., 1997]. Typically between 1 and 2mg of each GST-fusion protein was obtained and each protein was more than 75 judged by SDS polyacrylamide gel electrophoresis (data not shown).

PDK1 catalytic activity measurements

The ability of wild type and mutant PDK1 to phosphorylate the synthetic peptide T308tide (KTFCGTPEYLAPEVRR ([Biondi et al., 2000]) was carried out in 30 µl assays containing 100 ng of wild type or mutant PDK1, 50 mM Tris/HCl pH 7.5, 0.1% β -mercaptoethanol, 10 mM MgCl₂, 100 μM [32y P]ATP (200 cpm/pmol), 0.5 µM microcystin-LR, 1 mM T308tide in the presence or absence of the indicated concentrations of the S6K-pHM (SESANQVFLGFT(P)YVAPSV) S6K-HM.peptide peptide or (SESANQVFLGFTYVAPSV). After incubation for 10 min at 30 $^{\circ}$ C, 25 μl of the resultant mixture was spotted into P81 phosphocellulose paper (2 x 2 cm) and the papers washed and analysed as described previously for assays of MAP kinase. Control assays were carried out in parallel in which either PDK1, or peptide substrate were omitted; these values were always less than 5% of the activity measured in the presence of these reagents. One Unit of PDK1 activity was defined as that amount required to catalyse the phosphorylation of 1 nmol of the T308tide in 1 min.

Biacore analysis

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Binding was analysed in a BiaCore 3000 system (BiaCore AB, Stevenage, UK). Biotinylated S6K-pHM (Biotin-C₁₂- SESANQVFLGFT(P)YVAPSV) or the non-phosphorylated form of this peptide S6K-HM was bound to an streptavidin- coated Sensor chip (SA) (12 response units, RU). 30 μl of wild type or the indicated mutant GST-PDK1 were injected at a flow rate of 30μl/min, in buffer HBS-P (10 mM HEPES pH 7.4, 0.15M NaCl, 0.005% (by vol) polysorbate-20) supplemented with 1 mM DTT. Specific interactions between S6K-pHM and PDK1 proteins were obtained between the concentration range of 2-2150 nM PDK1. Steady state binding was

determined at each concentration. Dissociation of PDK1 from the phosphopeptide was monitored over a 1min period. Regeneration of the sensor chip surface was performed with 10 \(\pi\)µl injections of 0.05% SDS. As previously found for PDK1 binding to PIFtide [Biondi et al., 2000], the interaction data obtained using BiaCore did not fit to simple 1:1 interaction model. Apparent Kd values were estimated from the concentration of PDK1 which gives 50% of maximal response, which was obtained empirically using GST-PDK1[T148A] (RUmax=435). For all PDK1 construct tested, the off rates for S6Kp-HM were high in comparison to those of PIFtide binding with the time taken for 50% dissociation to occur for S6K-pHM is 30s compared to 1000s for PIFtide. This could account for the overall approximately 100-fold lower affinity of wild type PDK1 for S6K-pHM in comparison to PIFtide.

15 Data collection, structure solution, and refinement

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Data on PDK1 crystals were collected at the European Synchrotron Radiation Facility (Grenoble, France) beamline ID14-EH1, using an ADSC Q4 CCD detector. The temperature of the crystals was maintained at 100K using a nitrogen cryostream. Data were processed using the HKL package [Otwinowski and Minor, 1997], statistics are shown in Table I.

The structure of PDK1 was solved by molecular replacement with AMoRe [Navaza, 1994] using the structure of PKA in complex with an inhibitory peptide as a search model (PDB entry 1YDB), against 8-4 Ådata. A single, well separated solution was found with an R-factor of 0.479 (correlation coefficient = 0.428). The structure was automatically built using warpNtrace [Perrakis et al., 1999], which found 262 of a possible 309 residues, giving an initial protein model with R=0.293 (Rfree=0.318) after simulated annealing in CNS [Brunger et al., 1998]. Iterative protein

building in O [Jones et al., 1991] together with refinement in CNS, which included incorporation of a model for ATP, the phosphoserine in the activation loop, solvent molecules and a key sulphate molecule, resulted in a final model with R=0.195 (Rfree=0.222). No electron density was observed for residues 51-70 (the N-terminus of the construct) and 233-236 (the tip of the activation loop). All figures were made with PyMOL (http://www.pymol.org).

Table I

ATP

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Details of data collection & structure refinement for the PDK1 kinase domain. Values between brackets are for the highest resolution shell. All measured data were included in structure refinement.

	moustide data word moradod in sudden o formemons.						
	Wave length ()	0.933					
15	Space group	P3 ₂ 21					
	Unit cell ()	a=123.01, b=123.01, c=47.62					
	Resolution ()	25-2.0 (2.07-1.0)					
	Observed reflections	77315					
	Unique reflections	27643					
20	Redundancy ·	2.8 (2.5)					
	Completeness(%)	98.0 (93.5)					
	Rmerge	0.091 (0.454)					
	I/ sigma I	7.3 (2.0)					
	R _{free} reflections	579					
25	R _{cryst}	0.195					
	R_{free}	0.222					
	Number of groups	·					
	°°Protein residues	· 71-359					
	°°Water	200					

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	SO ₄	5
	Glycerol	8
	Wilson B (2)	22.4
•	Protein	25.6
5	Water	35.7
	< B > ATP	38.8
	RMSD from ideal geometry	
	Bond lengths ()	0.005
	Bond angles (°)	1.34
10	Main chain B (²)	1.5.

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Example 2: Co-ordinates for PDK1fragment with all alternate side chains.

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REMARK coordinates from restrained individual B-factor refinement
     REMARK refinement resolution: 25.0 - 2.0 A
     REMARK starting r= 0.1972 free_r= 0.2220
                    r= 0.1954 free_r= 0.2224
     REMARK final
     REMARK B rmsd for bonded mainchain atoms= 1.501 target= 1.5 REMARK B rmsd for bonded sidechain atoms= 2.235 target= 2.0
     REMARK B rmsd for angle mainchain atoms= 2.347 target= 2.0 REMARK B rmsd for angle sidechain atoms= 3.302 target= 2.5
     REMARK rweight= 0.0900 (with wa= 1.29263)
     REMARK target= mlf steps= 30
     REMARK sg= P3(2)21 a= 123.013 b= 123.013 c= 47.624 alpha= 90 beta= 90
     gamma= 120
     REMARK parameter file 1 : /ddl/david/projects/PDK1 new/CNS/prot.par
     REMARK parameter file 2 : /dd1/david/projects/PDK1_new/CNS/atp.par
REMARK parameter file 3 : CNS_TOPPAR:water_rep.param
REMARK parameter file 4 : CNS_TOPPAR:ion.param
REMARK parameter file 5 : /dd1/david/projects/PDK1_new/CNS/glycerol.par
15
     REMARK molecular structure file: ../generate/alternate.mtf
     REMARK input coordinates: ../minimize/minimize.pdb
     REMARK reflection file= ../../1/hkl/cns.hkl
     REMARK ncs= none
     REMARK B-correction resolution: 6.0 - 2.0
     REMARK initial B-factor correction applied to fobs :
               B11= -2.766 B22= -2.766 B33=
B12= -0.375 B13= 0.000 B23=
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     REMARK
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     REMARK
     REMARK B-factor correction applied to coordinate array B:
     REMARK bulk solvent: density level= 0.378441 e/A^3, B-factor= 52.6885 A^2
     REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
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	ATOM .	13	С	PRO A	72	57.527	-6.208	3.673	1.00	63.94	A
	ATOM	14	0	PRO A	72	56.710	-6.451	4.561		64.11	
	ATOM	15	N	ALA A	73	57.341	-5.268	2.753	1.00	61.57	Α
	ATOM	16	CA	ALA A	73	56.133	-4.454	2.708		58.74	
5	ATOM	17	CB	ALA A	73	56.438	-3.030	3.165		58.05	
	ATOM	18	С	ALA A	73	55.626	-4.448	1.271		56.78	
	ATOM	19	0	ALA A	73	56.347	-4.834	0.349		56.95	
	ATOM	20	N	PRO A	74	54.372	-4.024	1.057		54.15	
	ATOM	21	CD	PRO A	74	53.335	-3.610	2.018		53.31	
10	ATOM	22	CA	PRO A	74	53.856	-4.003	-0.314		52.54	
	ATOM	23	CB	PRO A	74	52.474	-3.375	-0.148		52.86	
	ATOM	24	CG	PRO A	74	52.067	-3.824	1.226		52.88	
	ATOM	25	С	PRO A	74	54.772	-3.167	-1.204		50.08	
	MOTA	26	0	PRO A	74	55.559	-2.361	-0.708		49.96	
15	ATOM	27	N	ALA A	75	54.680	-3.366	-2.514	1.00	47.58	A
	MOTA	28	CA	ALA A	75	55.503	-2.602	-3.446		44.69	
	ATOM	29	CB	ALA A	75	55.312	-3.121	-4.870		46.14	
	ATOM	30	C	ALA A	75	55.100	-1.134	-3.371		41.55	
	ATOM	31	0	ALA A	75	53.947	-0.813	-3.086		41.01	
20	MOTA	32	N	LYS A	76	56.053	-0.245	-3.619		38.31	
	MOTA	33	CA	LYS A	76	55.781	1.184	-3.588		35.72	
	MOTA	34	CB	LYS A	76	57.053	1.957	-3.930		37.70	
	ATOM.	35	CG	LYS A	76	57.123	3.356	-3.350		40.99	
	ATOM	36	CD	LYS A	76	57.262	3.316	-1.836		40.04	A
25	ATOM	37	CE	LYS A	76	57.511	4.705	-1.277		42.08	
	ATOM	38	NZ	LYS A	76	57.681	4.695	0.202		42.99	
	ATOM	39	С	LYS A	76	54.708	1.467	-4.638		32.65	
	MOTA	40	0	LYS A	76	54.814	1.005	-5.770		31.41	
	MOTA	41	N .	LYS A	77	53.668	2.207	-4.270		28.59	
30	MOTA	42	CA	LYS A	77	52.619	2.517	-5.232		25.72	
	AŢOM	43	CB	LYS A	77	51.316	2.865	-4.509		26.22	
	ATOM	44	CG	LYS A	.77	50.796	1.731	-3.631		27.15	
	ATOM	45	CD	LYS A	77	49.487	2.089	-2.967		26.80	
	ATOM	46	CE	LYS A	77	49.136	1.091	-1.870		27.31	
35	ATOM	47	NZ	LYS A	77	48.998	-0.296	-2.380		27.17	
	ATOM	48	C	LYS A	77	53.053	3.668	-6.137		24.67	
	ATOM .	49	.0	LYS A	77	54.010	4377	-5.829		21.60	
	MOTA	50	N	ARG A	78	52.351	3.838	-7.254		23.66	
	ATOM	51	CA	ARG A	78	52.662	4.897	-8.211		26.14	
40	MOTA	52	CB	ARG A	78	53.574	4.344	-9.318		28.57 34.78	
	ATOM	53	CG	ARG A	78	53.017		-10.050		40.96	
	ATOM	54	CD	ARG A	78	54.092		-10.896 -11.700		48.93	
	ATOM	55	NE	ARG A	78	53.560				52.58	
15	ATOM	56	CZ	ARG A	78	52.985		-11.203 -9.889		54.60	
45	ATOM	57		ARG A	78	52.860	0.113	-12.022		54.09	
	ATOM	58		ARG A	78	52.530		-8.803		23.76	
	ATOM	59	C	ARG A	78	51.382	5.488	-8.706		24.25	
	ATOM	60	0	ARG A	78	50.311	4.888	-9.428		21.76	
50	ATOM	61	И	PRO A	79	51.475 52.691	6.676 7.475	-9.668		20.82	
50 ·	ATOM .	62	CD	PRO A	79		•			21.96	
	ATOM	63	CA	PRO A	79	50.301		-10.021 -10.816		22.27	
	ATOM	64	CB	PRO A	79	50.910 52.124		-10.010		22.12	
	ATOM	65	CG	PRO A	79			-10.903		22.86	
55	ATOM	66 67	C	PRO A	79 79	49.446 48.213		-10.842		20.52	
55	ATOM	67 69	O N	PRO A GLU A	79 80	50.103		-11.714		21.87	
	ATOM	68 69	N		80	49.403		-12.628		22.99	
	ATOM	69 70	CB	GLU A		50.393	3.994 -1		0.50 2		AC1
	ATOM	70 _. 71	CG	GLU GLU		51.230	2.907 -3		0.50 2		AC1
	ATOM	1 T		GTO	30	J1.2J0	2.301 -		2.30 2		

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2.224 -13.913
                                                            0.50 31.99
     ATOM
              72
                   CD
                       GLU
                               80 52.157
                                            2.897 -14.433
                                                            0.50 34.34
                               80 53.072
     MOTA
              73
                   OE1 GLU
                                                                         AC1
                                            1.015 -14.172
                                                            0.50 32.83 AC1
     ATOM
              74
                   OE2 GLU
                               80 51.969
                                              3.631 -11.912
                                                              1.00 22.09
              75
     ATOM
                   С
                       GLU A
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                                    48.556
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                                              3.013 -12.530
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                                              2.423 -9.874
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                                                                            Α
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                                                                            Α
                   CB
                       ASP A
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                               81
                       ASP A
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                                                                            Α
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                                                 1.685
                                                        -8.058
                                                                  1.00 23.33
     ATOM
              82
                   OD2 ASP A
                               81
                                                         -9.518
                                                                  1.00 20.85
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                               81
                                        46.652
                                                 2.975
                                                                                   Α
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                                                         -9.015 - 1.00 19.96
                                       45.793
                                                 2.246
     MOTA
              84
                   0
                       ASP A
                               81
                                                                                   A
                                       46.445
                                                 4.258
                                                         -9.804
                                                                  1.00 18.91
                                                                                   Α
                       PHE A
                               82
     ATOM
              85
                   N
                                                         -9.465
                                                                  1.00 19.30
15
                       PHE A
                               82
                                        45.200
                                                 4.934
                                                                                   Α
              86
                   CA
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              87
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                                        45.475
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                                                         -7.175
                                                                  1.00 18.01
                                                                                   Α
     ATOM
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                   CG
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                                                                  1.00 17.19
                                                                                   Α
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                                                                  1.00 18.99
                                                                                   Α
              90
                   CD2 PHE A
                               82
                                        47.520
                                                 5.460
     MOTA
                               82
                                       45.977
                                                 4.676
                                                         -4.918
                                                                  1.00 17.12
                                                                                   Α
20
    ATOM
              91
                   CE1 PHE A
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                   CE2
                       PHE A . 82
                                        48.137
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                                                                                   Α
     MOTA
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                               82
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                                                                                   A
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                                                 5.596 -10.621
                                                                                   Α
                                        44.476
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                   С
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                                                                                   Α
                       PHE A
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              95
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                               82
                                                 5.792 -10.411
                                                                  1.00 19.80
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                       LYS A
                               83
                                        43.182
25
                   N
     MOTA
                                        42.321
                                                 6.478 -11.353
                                                                  1.00 21.65
                                                                                   Α
              97
                       LYS A
                               83
     ATOM
                   CA
                                                                                   Α
                                                                  1.00 22.02
     ATOM
               98
                   CB
                       LYS A
                               83
                                        41.096
                                                 5.625 -11.687
                                                                  1.00 28.93
                                                                                   Α
                                        40.062
                                                 6.326 -12.550
     ATOM
               99
                   CG
                       LYS A
                              '83
                                                                                   Α
                                        38.974
                                                 5.355 -12.981
                                                                  1.00 34.20
                       LYS A
     MOTA
             100
                   CD
                               83
                                        37.909
                                                 6.042 -13.824
                                                                  1.00 38.10
                                                                                   Α
30
                       LYS A
                               83
     ATOM
             101
                   CF.
                                                                  1.00 43.33
     ATOM
             102
                   NZ
                       LYS A
                               83
                                        37.179
                                                 7.086 -13.043
                                                                                   Α
                                                 7.702 -10.541
                                                                  1.00 20.74
                                        41.913
                                                                                   Α
              103
                       LYS A
                               83
     ATOM
                   С
                                        41.084
                                                 7.606 -9.635
                                                                  1.00 20.98
                       LYS A
     MOTA
             104
                   0
                               83
                                                 8.848 -10.835
                                                                  1.00 19.99
                                                                                   Α
                               84
                                        42.513
             105
                       PHE A
     MOTA
                   N
                                                                                   Α
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                       PHE A
                               84
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                                                                                   Α
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             107
                   CB
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                                                10.741
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                                                                  1.00 17.68
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             108
                   CG
                       PHE A
                               84
                                       44.571
     ATOM
                                                                  1.00 18.16
                                                                                   A
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                                                 9.926 -10.224
     ATOM
             109
                   CD1 PHE A
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                                        44.843
                                                         -8.299
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                                                                                   Α
                                                11.183
                   CD2 PHE A
                               84
     ATOM
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                                                                  1.00 18.09
40
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                   CE1 PHE A
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                                                                  1.00 18.89
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                                                                                    Α
                                                         -7.653
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                                                10.816
     MOTA
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     MOTA
              113
                   CZ
                       PHE A
                               84
                                                                  1.00 19.69
                                                                                    Α
                       PHE A
                               84
                                        40.834
                                                10.617 -10.460
     ATOM
             114
                   С
                                                                                    Α
                                        40.391
                                                10.489 -11.601
                                                                  1.00 20.72
     ATOM
             115
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                       PHE A
                               84
                                                                  1.00 16.80
                                                                                   Α
             116
                                        40.178
                                                11.233
                                                        -9.484
45
     ATOM
                   N
                       GLY A
                               85
                                                                                   Α
                                                         -9.716
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                       GLY A
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                                        38.872
                                                11.810
     ATOM
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                       GLY A
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                       GLY A
                               85
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                   0
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     MOTA
             120
                   N
                       LYS A
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                                        37.753
                                                13.673
                                                         -8.659
                                                                  1.00 16.00
                                                                                    Α
                                                                  1.00 18.26
                                                                                    Α
                       LYS A
                               86
                                        37.571
                                                15.064
                                                         -8.278
     ATOM
             121
                   CA
                                        36.133
                                                15.302
                                                         -7.812
                                                                  1.00 19.00
                                                                                   Α
     ATOM
             122
                       LYS A
                               86
                   CB
                                                                                    Α
                                        35.793
                                                14.660
                                                         -6.481
                                                                  1.00 21.55
     ATOM
             123
                   CG
                       LYS A
                               86
                                                                                   A
                       LYS A
                                        34.368
                                                14.981
                                                         -6.066
                                                                  1.00 26.48
                               86
     MOTA
             124
                   CD
                                                                  1.00 31.92
                                                                                   Α
                       LYS A
                               86
                                       33.994
                                                14.239
                                                         -4.793
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             125
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                                                                                   Α
                                                                  1.00 35.36
                               86
                                        32.568
                                                14.457
                                                         -4.412
     ATOM
             126
                   NZ
                       LYS A
                                                         -7.202
                                                                  1.00 18.57
                                                                                    Α
                                                15.571
                                        38.523
     ATOM
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                   С
                       LYS A
                               86
                               86
                                        39.045
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                                                         -6.385
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                       LYS A
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                                                                                   A
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                       ILE A
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                                                16.881
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                                                         -6.256
                                                                  1.00 18.26
     ATOM
             130
                   CA
                       ILE A
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	ATOM	131	СВ	ILE	А	87		39.994	18.952	-6.772	1.00 19.60	Α
	ATOM	. 132		ILE		87		40.593	19.786	-5.628	1.00 18.73	A
	ATOM	133		ILE		87		40.968	18.786	-7.945	1.00 21.16	A
	ATOM	134		ILE		87		41.412	20.087	-8.588	1.00 25.26	A
5	ATOM	135	C	ILE		87		38.731	17.709	-4.997	1.00 19.67	A
,	ATOM	136	ō	ILE		87		37.628	18.249	-5.052	1.00 20.41	A
		137	N	LEU		88		39.240	17.229	-3.867	1.00 19.15	A
	ATOM					88		38.508	17.324	-2.611	1.00 20.68	A
	ATOM	138	CA	LEU				38.870	16.151	-1.700	1.00 20.00	A
••	MOTA	139	CB	LEU		88		38.529	14.759	-2.237	1.00 19.37	A
10	MOTA	140	CG	LEU		88					1.00 19.24	A
	ATOM	141		LEU		88		39.090	13.692	-1.311		A
	ATOM	142		LEU		88		37.029	14.622	-2.359	1.00 18.84	
	MOTA	143	С	LEU		88		38.815	18.632	-1.901	1.00 23.11	A
	ATOM	144	Q	LEU		88		37.999	19.146	-1.139	1.00 25.10	A
15	ATOM	145	N	GLY		89		39.997	19.174	-2.149	1.00 24.09	A
	ATOM '	146	CA	GLY		89		40.367	20.418	-1.507	1.00 24.27	A
	ATOM	147	С	GLY		89		41.658	20.954	-2.078	1.00 25.47	A
	ATOM	148	0	GLY	A	89		42.445	20.202	-2.666	1.00 22.19	A
	ATOM	149	N	${ t GLU}$	Α	90		41.870	22.254	-1.906	1.00 26.22	Α
20	ATOM	150	CA	GLU	Α	90		43.064	22.924	-2.404	1.00 29.96	Α
	MOTA	151	CB	GLU	Α	90		42.698	23.814	~3.596	1.00 30.75	A
	ATOM	152	CG	GLU	A	90 -		42.267	23.038	-4.831	1.00 34.32	A
	ATOM	153	CD	GLU	Α	90		41.711	23.930	-5.927	1.00 38.27	A
	ATOM	154	OE1	GLU	Α	90		40.590	24.456	-5.764	1.00 40.57	. A
25	ATOM	155		GLU		90		42.398	24.110	-6.952	1.00 40.90	A
	ATOM	156	С	GLU	Α	90		43.711	23.768	-1.313	1.00 30.68	A
	ATOM	157	0	GLU		90		43.049	24.574	-0.668	1.00 32.83	A
	ATOM	158	N	GLY		91		45.006	23.566	-1.104	1.00 29.66	A
	ATOM	159	CA	GLY		91		45.724	24.332	-0.104	1.00 29.40	A
30	ATOM	160	C	GLY		91		46.795	25.151	-0.798	1.00 29.98	A
20	ATOM	161	ō	GLY		91		46.894	25.130	-2.028	1.00 28.16	A
	ATOM	162	N	SER		92		47.605	25.870	-0.029	1.00 28.30	·A
	ATOM	163	CA	SER		92		48.653	26.681	-0.633	1.00 30.50	A
	ATOM	`164	CB	SER		92		49.165	27.717	0.370	1.00 32.43	A
35	ATOM	165	OG	SER		92		49.520	27.099	1.593	1.00 40.94	A
55	ATOM	166	C	SER		92		49.815	25.843	-1.164	1.00 29.77	A
	ATOM	167	Ö	SER		92		50.456	26.221	-2.143	1.00 30.46	Ä
	ATOM	168	N		A	93		50.087	24.703	-0.536	1.00 27.65	. A
	ATOM	169	CA	PHE		93		51.185	23.855	-0.995	1.00 26.34	A
40		170	CB		A	93		52.281	23.785	0.068	1.00 27.95	A
40	ATOM ATOM	171	CG		A	93		52.861	25.117	0.406	1.00 31.06	A
		172		PHE		93		52.283	25.909	1.392	1.00 29.96	Α
	ATOM	173			A	93		53.949	25.613	-0.308	1.00 31.38	Α
	ATOM			PHE		93		52.779	27.181	1.665	1.00 32.69	А
4.5-	ATOM	174				93		54.452	26.883	-0.044	1.00 32.63	A
45	ATOM	175		PHE				53.864	27.670	0.945	1.00 31.81	• A
	ATOM	176	CZ	PHE		93		50.759	22.445	-1.365	1.00 25.39	A
	ATOM	177	C	PHE		93		51.601	21.559	-1.522	1.00 24.59	A
	ATOM	178	0	PHE		93			22.235	-1.519	1.00 23.63	A
	ATOM	179	N	SER		94		49.457		-1.860	1.00 23.03	A
50	ATOM	180	CA	SER		94		48.965	20.912	-0.628	1.00 21.43	A
	ATOM	181	CB	SER		94		49.017	20.013 20.475		1.00 21.42	. A
	ATOM	182	OG	SER		94		48.091		0.340	1.00 21.19	. A
	ATOM '	183	C	SER		94	•	47.539	20.925	-2.378 -2.173	1.00 19.82	A
	ATOM	184	0	SER		94		46.795	21.882	-2.173	1.00 18.76	A
55	ATOM	185	N	THR		95		47.174	19.832	-3.038		A
	ATOM	186	CA	THR		95		45.840	19.637	-3.580	1.00 17.98	A
	MOTA	187	СВ	THR		95		45.818	19.818	-5.110	1.00 19.25	A
	ATOM	188		THR		95		46.196	21.162	-5.434	1.00 22.04	A
	MOTA	189	CG2	THR	A	95		44.421	19.549	-5.661	1.00 17.61	, н
												*

	ATOM	190	C ·	THR	Α	95		45.455	18.201	-3.243	1.00 18.	61	A
	ATOM	191	o ·	THR	Α	95		46.212	17.264	-3.524	1.00 17.		A
	ATOM	192	N	VAL		96		44.295	18.024	-2.623	1.00 16.		A
	ATOM	193	CA	VAL		96		43.845	16.685	-2.266			
_											1.00 16.		A
5	ATOM	194	CB	VAL		96		43.170	16.672	-0.886	1.00 16.		A
	ATOM	195		VAL		96		42.741	15.249	-0.532	1.00 18.		Α
	ATOM	196	CG2	VAL	Α	96		44.145	17.206	0.168	1.00 16.	69	Α
	ATOM	197	С	VAL	Α	96		42.875	16.207	-3.335	1.00 16.	42	Α
	ATOM	198	0	VAL	Α	96		41.906	16.892	-3.665	1.00 16.	47	A
10	ATOM	199	N	VAL	Α	97		43.157	15.033	-3.888	1.00 16.	80	A
	ATOM	200	CA	VAL		97		42.338	14.471		1.00 16.		Α
	ATOM	201	СВ	VAL		97		43.153	14.354	-6.255	1.00 18.		A
	ATOM	202		VAL		97		42.249	13.927	-7.404	1.00 19.		A
				VAL		97		43.831	15.685	-6.569	1.00 17.		A
1.5	ATOM	203											
15	ATOM	204	С	VAL		97		41.812	13.091	-4.583	1.00 16.		A
	MOTA	205	0	VAL		97		42.532	12.270	-4.014	1.00 17.		Α
	MOTA	206	N	LEU	Α	98		40.545	12.845	-4.895	1.00 16.	62	Α
	ATOM	207	CA	$_{ m LEU}$	Α	98		39.947	11.548	-4.624	1.00 17.	04	Α
	ATOM	208	CB	LEU	Α	98		38.424	11.633	-4.743	1.00 16.	89	Α
20	MOTA	209	CG	LEU	Α	98		37.635	10.342	-4.508	1.00 19.	46	Α
	ATOM	210		LEU		98		37.990	9.762	-3.146	1.00 20.	07	Α
	ATOM	211	-	LEU		98		36.143	10.627	-4.588	1.00 17.		Α
	ATOM	212	C	LEU		98		40.512	10.597	-5.677	1.00 17.		A
			•					40.527	10.920	-6.863	1.00 18.		A
0.5	ATOM	213	0	LEU		98	•						'A
25	ATOM	214	N	ALA		99		40.995	9.438	-5.246	1.00 17.		
	ATOM	215	CA	ALA		99		41.570	8.466	-6.168	1.00 18.		A
	ATOM	216	CB	ALA	A	99		43.090	8.524	-6.105	1.00 14.		A
	MOTA	217	C	ALA	A	99		41.102	7.055	-5.848	1.00 21.		Α
	ATOM	218	0	ALA	Α	99		40.941	6.691	-4.679	1.00 22.	52	Α
30	MOTA	219	N	ARG	Α	100		40.878	6.261	-6.888	1.00 19.	77	Α
	ATOM	220	CA	ARG	Α	100		40.459	4.884	-6.693	1.00 20.	85	Α
	ATOM	221	СВ	ARG				39.202	4.585	-7.518	1.00 24.	22	Α
	ATOM	222	CG	ARG				38.608	3.205	-7.256	1.00 31.	78	A
	ATOM	223	CD	ARG				37.326	2.979	-8.048	1.00 36.		Α
35		224		ARG				36.213	3.818	-7.594	1.00 41.		A
33	ATOM		NE						3.662	-6.439	1.00 42.		A
	ATOM	225	CZ	ARG				35.566			1.00 42.		A
	ATOM	226		ARG				35.912	2.696	-5.598			
	ATOM	227		ARG				34.559	4.468	-6.128	1.00 43.		A
	ATOM	228	С	ARG				41.613	3.985	-7.129	1.00 18.		A
40	ATOM	229	0	ARG	Α	100		42.078	4.065	-8.271	1.00 19.		A
	MOTA	230	N	GLU	Α	101		42.102	3.157	-6.212	1.00 16.	43	A
	ATOM	231	.CA	GLU	Α	101		43.196	2.246	-6.533	1.00 16.	11	Α
	ATOM	232	СВ	GLU	Α	101		43.774	1.637	-5.248	1.00 16.	79	A
	ATOM		CG	GLU	Α	101		44.917	0.657	-5.488	1.00 16.	51	A
45	ATOM	234	CD	GLU				45.501	0.115	-4.200	1.00 18.	20	Α
73	MOTA	235		GLU	70	101		44.733		3.239	1.00 18.		Α
		236		GLU				46.725	-0.132	-4.150	1.00 17.		A
	ATOM										1.00 17.		A
	ATOM	237	C	GLU				42.625	1.152	-7.442			
	ATOM	238	0	GLU				41.681	0.462	-7.069	1.00 18.		A
50 -	ATOM	239	N	LEU				43.198	1.002	-8.632	1.00 19.		A
	ATOM	240	CA	LEU				42.718	0.025	-9.607	1.00 20.		A
•	ATOM	241	CB	LEU	A	102		43.569		-10.878	1.00 23.		A
	ATOM	242	CG	LEU	Α	102		43.531	1.426	-11.642	1.00 25.		A
	ATOM	243		LEU				44.577	1.414	-12.748	1.00 27.	88	Α
55	ATOM	244		LEU				42.140		-12.214	1.00 26.	79	Α
	ATOM	245	C	LEU				42.671	-1.418	-9.125	1.00 21.		Α
	ATOM	246	ŏ	LEU				41.668	-2.103	-9.305	1.00 21.		A
		247	N	ALA				43.753	-1.874	-8.507	1.00 19.		A
	ATOM			ALA				43.733	-3.249	-8.035	1.00 20.		Α
	ATOM	248	CA	MIN	м	103		33.030	-2.643	0.000	1.00 20.		••

	ATOM	249	CB	ALA	A 1)3	45.284	-3.571	-7.671	1.00 19.23	A
	ATOM	250	С	ALA	A 10)3	42.919	-3.629	-6.872	1.00 19.92	Α
	ATOM	251	0	ALA			42.703	-4.815	-6.628	1.00 20.38	A ·
		252									
_	ATOM		N		A 10		42.361	-2.643	-6.175	1.00 18.12	A
5	ATOM	253	CA		A 10		41.517	-2.927	5.018	1.00 17.15	A
	ATOM	254	CB	THR	A 1)4	42.212	-2.484	-3.717	1.00 19.54	A
	ATOM	255	OG1	THR	A 10)4	42.456	-1.070	-3.773 [°]	1.00 19.26	A.
	ATOM	256		THR			43.536	-3.219	-3.529	1.00 17.02	A
		257	C								
••	ATOM				A 10		40.159	-2.247	-5.026	1.00 19.44	. A
10	ATOM	258	0		A 10		39.259	-2.648	-4.285	1.00 18.70	A
	MOTA	259	N	SER	A 10)5	40.034	-1.207	-5.847	1.00 19.65	A
	MOTA	260	CA	SER	A 10)5	38.819	-0.400	-5.967	1.00 19.37	A
	ATOM	261	CB	SER	10		37.598	-1.304	-6.173	0.50 21.81	AC1
	ATOM	262	OG	SER	10		36.431			0.50 23.01	
1.5								-0.539	-6.412		AC1
15	ATOM	263	С		A 10		38.644	0.447	-4.701	1.00 18.99	A
	ATOM	264	0	SER	A 10)5	37.602	1.070	-4.488	1.00 18.66	Α
	ATOM .	265	N	ARG	A 10	6 .	39.674	0.468	-3.861	1.00 16.84	Α
	ATOM	266	CA	ARG	A 10	6	39.655	1.267	-2.634	1.00 16.21	A
	ATOM	267	СВ	ARG			40.827	0.886	-1.723	1.00 16.41	A
20											
20	ATOM	268	CG	ARG			40.619	-0.367	-0.906	1.00 15.49	A
	ATOM	269	CD	ARG			41.887	-0.755	-0.170	1.00 17.43	A
	ATOM	270	NE	ARG	A 10	6	41.620	-1.792	0.824	1.00 20.47	A
	ATOM	271	CZ	ARG	A 10	6	42.548	-2.568	1.371	1.00 20.24	· A
	ATOM	272		ARG		6	43.821	-2.433	1.017	1.00 17.80	A
25						- /					
23	ATOM	273		ARG			42.198	-3.468	2.285	1.00 20.14	A
	ATOM	274	С	ARG			39.785	2.746	-2.981	1.00 17.37	A
	MOTA	275	0	ARG	A 10	6	40.514	3.103	-3.902	1.00 17.75	Α
	ATOM	276	N	GLU	A 10	7	39.085	3.599	-2.240	1.00 16:06	A
	ATOM	277	CA	GLU	A 10	7	39.156	5.039	-2.461	1.00 20.80	A
30	ATOM	278	СВ	GLU			37.779	5.694	-2.337	1.00 22.93	A
50											
	ATOM	279	CG	GLU			36.711	5.171	-3.269	1.00 30.87	A
	ATOM	280	CD	\mathtt{GLU}			35.431	5.975	-3.148	1.00 32.40	A
	ATOM	281	OE1	GLU	A 10	7	35.262	6.939	-3.923	1.00 33.74	Α
	ATOM	282	OE2	GLŲ	A 10	7	34.608	5.654	-2.263	1.00 36.00	A
35	ATOM	283	С.				40.053	5.678	-1.410	1.00 18.93	Α
	ATOM	284	o .	GLU			39.891	5.427	-0.220	1.00 19.21	A
	ATOM	285	N	TYR			40.988	6.507	-1.852	1.00 16.70	A
	ATOM	286	CA	TYR			41.883	7.209	-0.942	1.00 15.86	A
	ATOM	287	CB	TYR	A 10	8	43.325	6.728	-1.104	1.00 15.30	Α
40	ATOM	288	CG	TYR	A 10	8	43.593	5.328	-0.612	1.00 16.33	Α
	ATOM .	289	CD1	TYR			43.765	5.066	0.746	1.00 16.36	A
	ATOM	290		TYR			44.046	3.769	1.201	1.00 18.48	A
	ATOM	291		TYR			43.701	4.268	-1.511	1.00 13.25	. A
	ATOM	292		TYR			43.980	2.981	-1.075	1.00 17.28	A
45	ATOM	293	CZ	TYR	A 10	8	44.152	2.736	0.276	1.00 19.17	A
	ATOM	294	OH	TYR			44.440	1.461	0.688	1.00 19.38	A
	ATOM	295	C	TYR			41.850	8.687	-1.292	1.00 16.80	A
	ATOM										
		296	0	TYR			41.560	9.058	-2.431	1.00 15.22	A
	ATOM	297	N	ALA			42.132	9.528	-0.306	1.00 14.61	A
50	ATOM	298	CA	ALA .	A 10	9	42.207	10.957	-0.539	1.00 14.30	A
	ATOM	299	CB	ALA	A 10	9	41.671	11.726	0.661	1.00 14.78	A `
	ATOM	300	С	ALA			43.713	11.136	-0.667	1.00 16.79	Α
	ATOM	301	Ö	ALA			44.450	10.983	0.317	1.00 16.73	A
										· ·	
	ATOM	302	N	ILE			44.182	11.410	-1.881	1.00 14.80	A
55	ATOM	303	CA	ILE			45.609	11.574	-2.093	1.00 15.80	A
	ATOM	304	CB	ILE	A 11	0	46.065	10.863	-3.396	1.00 16.85	A
	ATOM	305	CG2	ILE .			47.550	11.098	-3.632	1.00 16.80	A
	ATOM	306		ILE			45.774	9.358	-3.284	1.00 17.76	A
	ATOM	307		ILE					-4.437	1.00 17.70	A
	AI OH	507	CDI	THE.	u TT	U	46.308	8.513	-4.43/	1.00 10.07	A

								•	•		
	ATOM	308	С	ILE	Α	110	46.004	13.045	-2.129	1.00 17.78	A
	ATOM	309	0	ILE	Α	110	45.534	13.813	-2.976	1.00 16.24	·A
	ATOM	310	N	LYS	Α	111	46.846	13.435	-1.177	1.00 16.15	A
	ATOM	311	CA	LYS	Α	111	47.326	14.808	-1.100	1.00 17.20	A
5	ATOM	312	CB	LYS	Α	111	47.700	15.176	0.344	1.00 17.41	A
	ATOM	313	CG	LYS	Α	111	48.350	16.547	0.464	1.00 20.71	A
	ATOM	314	CD	LYS	Α	111	48.585	16.971	1.910	1.00 24.25	A
	ATOM	315	CE			111	47.288	17.381	2.598	1.00 29.46	A
	ATOM	316	NZ			111	47.516	17.866	4.000	1.00 30.50	A
10	ATOM	317	С			111	48.551	14.890	-1.994	1.00 16.41	A
	ATOM	318	0			111	49.509	14.137	-1.813	1.00 18.20	A
	ATOM	319	N			112	48.509	15.798	-2.963	1.00 15.87	A
	ATOM	320	CA			112	49.606	15.967	-3.907	1.00 17.28	A
-	ATOM	321	CB			112	49.079	15.911	-5.358	1.00 16.43	A
15	ATOM	322	CG2			112	50.235	15.998	-6.341	1.00 15.12	A
	ATOM	323		ILE			48.293	14.609	-5.565	1.00 16.82	A
	ATOM	324		ILE			47.580	14.511	-6.904	1.00 18.47	A
	ATOM	325	C			112	50.307	17.301	-3.663	1.00 19.03	A
	ATOM	326	Ö			112	49.669	18.350	-3.635	1.00 19.15	A
20	ATOM	327	N			113	51.622	17.245	-3.472	1.00 20.22	. A
	ATOM	. 328	CA			113	52.416	18.442	-3.214	1.00 22.36	A
	ATOM	329	CB			113	52.995	18.397	-1.794	1.00 22.13	A
	ATOM	330	CG			113	52.042	18.063	-0.646	1.00 22.46	A
	ATOM	331		LEU			51.866	16.557	-0.553	1.00 23.81	A
25	MOTA	332		LEU			52.603	18.595	0.660	1.00 23.68	A
	ATOM	333	C			113	53.560		-4.215	1.00 23.37	A
	ATOM	334	ō			113	54.300	17.586	-4.424	1.00 23.11	A
	ATOM	335	N			114	53.706	19.714	-4.834	1.00 23.88	A
	MOTA	336	CA			114	54.771	19.920	-5.806	1.00 26.00	
30	ATOM	337	CB			114	54.435	21.111	-6.706	1.00 27.74	A
	MOTA	338	CG	GLU	A	114	55.533	21.452	-7.696	1.00 35.07	A
	ATOM	339	CD	GLU	Α	114	55.220	22.696	-8.497	1.00 39.24	Α
	ATOM	340	OE1	GLU	Α	114	54.808	23.703	-7.885	1.00 41.45	A
	ATOM	341	OE2	GLU	Α	114	55.395	22.670	-9.736	1.00 44.05	A
35	MOTA	342	С	GLU	Α	114	56.087	20.163	-5.067	1.00 24.37	Α
	ATOM	343	0	GLU	A	114	56.186	21.071	-4.238	1.00 24.43	A
	MOTA	344	N .	LYS	Α	115	57.096	19.350	-5.360	1.00 24.10	A
	MOTA	345	CA	LYS	Α	115	58.376	19.493	-4.678	1.00 24.93	A
	ATOM	346	CB	LYS	Α	115	59.339	18.373	-5.103	1.00 23.72	A
40	ATOM	347	CG			115	59.139	17.080	-4.308	1.00 23.09	A
	ATOM	348	CD	LYS			60.064	15.944	-4.743	1.00 21.92	A
•	ATOM	349	CE			115	59.691	15.400	-6.117	1.00 22.42	A
	ATOM	350	ΝZ			115	60.447	14.150	-6.448	1.00 19.71	A
	ATOM	351	С	LYS			59.031	20.858	-4.868	1.00 26.87	A
45	MOTA	352	0	LYS			59.492	21.469	-3.903	1.00 26.17	A
	ATOM ·	353	N	ARG			59.058	21.348	-6.102	1.00 28.73	A
	MOTA	.354	CA	ARG	Α		59.678	22.638	-6.380	1.00 29.66	A
	ATOM	355	CB	ARG		116	59.533	22.980	-7.868	0.50 31.29	AC1
	MOTA	356	CG	ARG		116	60.047	24.361	-8.267	0.50 33.19	AC1
50	ATOM	357	CD	ARG		116	61.368	24.710	-7.590	0.50 35.13	AC1
	MOTA	358	NE	ARG		116	62.329	23.612	-7.618	0.50 36.42	AC1
	MOTA	359	CZ	ARG		116	63.510	23.648	-7.009	0.50 36.18	AC1
	ATOM	360		ARG		116	63.871	24.729	-6.332	0.50 36.12	AC1
E E	ATOM	361	NH2		_	116	64.324	22.602	-7.067	0.50 35.77	AC1
55	ATOM	362	C	ARG			59.097	23.761	-5.519	1.00 29.70	A
	ATOM	363	0	ARG			59.843	24.515	-4.889	1.00 29.16	A
	ATOM	364	N	HIS			57.773	23.862	-5.472	1.00 27.22	A
	MOTA	365 366	CA	HIS			57.126	24.903	-4.681	1.00 26.33	A
	ATOM	366	CB	HIS	А	TT \	55.606	24.835	-4.848	1.00 28.41	A

	ATOM	367	CG	HIS	A	117		54.881	26.005	-4.258	1.00 31.82	A
	ATOM	368	CD2	HIS	Α	117		55.309	27.249	-3.935	1.00 33.19	· A
	ATOM	369	ND1	HIS	A	117		53.536	25.974	-3.961	1.00 34.30	A
	ATOM	370	CE1	HIS	Α	117		53.165	27.148	-3.480	1.00 34.58	. A
5	ATOM	371	NE2	HIS	Α	117		54.222	27.940	-3.455	1.00 35.18	· A
	ATOM	372	C	HIS	Α	117		57.477	24.780	-3.202	1.00 26.22	Α
	ATOM	373	.0	HIS	Α	117		57.737	25.776	-2.534	1.00 25.67	A.
	ATOM	374	N	ILE	Α	118		57.469	23.554	-2.689	1.00 24.94	A
	ATOM	375	CA	ILE	Α	118		57.792	23.315	-1.285	1.00 23.94	A
10	ATOM	376	CB	ILE	Α	118		57.711	21.812	-0.952	1.00 23.50	A
	ATOM	377	CG2	ILE	Α	118		58.374	21.533	0.389	1.00 23.76	· А
	ATOM	378	CG1	ILE	Α	118 '		56.246	21.362	-0.959	1.00 24.42	A
	ATOM	379	CD1	ILE	Α	118		56.066	19.858	-0.834	1.00 28.06	A
	ATOM	380	С	ILE	Α	118		59.195	23.821	-0.958	1.00 23.78	A
15	ATOM	381	0	ILE	Α	118		59.402	24.495	0.048	1.00 23.49	A
	ATOM	382	N	ILE	Α	119		60.153	23.489	-1.815	1.00 23.46	A
	ATOM	383	CA	ILE	A	119		61.534	23.913	-1.619	1.00 25.13	A
	ATOM	384	CB	ILE	Α	119		62.467	23.250	-2.664	1.00 24.25	A
	ATOM	385	CG2	ILE	Α	119		63.858	23.890	-2.617	1.00 22.47	A
20	ATOM	386	CG1	ILE	Α	119		62.540	21.738	-2.395	1.00 25.05	A
	ATOM	387	CD1	ILE	Α	119		63.327	20.945	-3.439	1.00 24.62	Α
	ATOM	388	С	ILE	A	119		61.667	25.435	-1.705	1.00 25.96	A
	ATOM	389	0	ILE	Α	119		62.330	26.051	-0.872	1.00 24.78	A
	ATOM	390	N	LYS	A	120		61.028	26.039	-2.704	1.00 27.67	A
25	ATOM	391	CA	LYS	Α	120		61.100	27.489	-2.879	1.00 30.29	A
	ATOM	392	CB	LYS	A	120		60.242	27.940	-4.060	1.00 32.34	A
	MOTA	393	CG	LYS	A	120		60.674	27.407	-5.409	1.00 39.30	A
	ATOM	394	CD	LYS	Α	120		59.765	27.950	-6.512	1.00 45.19	A
	ATOM	395	CE ·					58.294	27.636	-6.218	1.00 46.48	A
30	ATOM	396	NZ	LYS				57.363	28.155	-7.252	1.00 46.49	A
	ATOM	397	С	LYS				60.647	28.247	-1.638	1.00 30.89	A
	ATOM	398	0	LYS				61.303	29.198	-1.217	1.00 32.48	A
	ATOM	399	N	GLU				59.527	27.825	-1.055	1.00 29.82	A
	ATOM	400	CA	GLU				58.986	28.488	0.128	1.00 30.33	A
35	MOTA	401	CB	GLU				57.455	28.416	0.117	1.00 33.04	A
	ATOM	402	CG	GLU				56.794	29.021	-1.120	1.00 36.45	. A
	ATOM	403	CD	GLU				57.221	30.456	-1.373	1.00 39.88	A
	ATOM	404		GLU				57.200	31.264	-0.420	1.00 40.53	A
40	ATOM	405		GLU			•	57.573	30.778	-2.529	1.00 43.24 1.00 30.37	A A
40	ATOM	406	C	GLU				59.511	27.930	1.451 - 2.513	1.00 30.37	A
	ATOM	407	0	GLU ASN				58.946 60.588	28.204 27.151	1.390	1.00 31.24	A
	ATOM	408	N					61.183	26.573	2.594	1.00 29.03	A
	ATOM	409	CA	ASN				61.836	27.673	3.436	1.00 28.40	Ā
45	ATOM	410	CB	ASN ASN				62.945	28.395	2.698	1.00 31.20	A
. 45	ATOM	411	CG	ASN				62.697	29.143	1.754	1.00 34.12	· A
	MOTA	412						64.181		3.127	1.00 35.73	A
	ATOM ATOM	413 414	C	ASN ASN				60.157	25.835	3.456	1.00 26.89	A
		415	0	ASN				60.085	26.055	4.663	1.00 27.23	A
50	ATOM ATOM	416	N	LYS				59.375	24.955	2.842	1.00 27.23	A
. 50	ATOM	417	CA	LYS				58.358	24.210	3.574	1.00 23.33	A
	ATOM	418	CB	LYS				57.031	24.248	2.810	1.00 21.97	A
	ATOM	419	CG	LYS				56.475	25.645	2.599	1.00 25.68	
	ATOM	420	CD	LYS				56.253	26.354	3.927	1.00 27.54	A
55	ATOM	421	CE	LYS				55.822	27.796	3.716	1.00 27.34	A
<i></i>	ATOM	422	NZ	LYS				55.756	28.540	5.004	1.00 33.21	A
	ATOM	423	C	LYS				58.748	22.759	3.821	1.00 22.20	A
	ATOM	424	Õ	LYS				57.924	21.960	4.264	1.00 22.50	A
	ATOM	425	N	VAL				59.997	22.412	3.535	1.00 20.59	A
	224 012	725	.,	4 7-177		1		,				

	ATOM	426	CA	VAL	Α	124	60.439	21.039	3.730	1.00	20.25	A
	ATOM .	427	СВ	VAL	Α	124	61.922	20.850	3.328		19.43	· A
	ATOM	428	CG1	VAL	Α	124	62.346	19.407	3.573	1.00	18.69	A
	ATOM	429	CG2	VAL	A	124	62.104	21.195	1.853	1.00	18.21	A
5	ATOM	430	С	VAL	Α	124	60.236	20.561	5.163	1.00	19.53	A
	ATOM	431	0	VAL			59.841	19.418	5.385		20.02	A
	MOTA	432	N	PRO	Α	125	60.513	21.422	6.159		20.01	A
	ATOM	433	CD	PRO	Α	125	61.178	22.738	6.118	1.00	18.69	A
	ATOM	434	CA	PRO	Α	125	60.318	20.979	7.544		19.88	A
10	ATOM	435	CB	PRO			60.793	22.180	8.363		19.95	A
	ATOM	436	CG	PRO			61.839	22.805	7.479		18.85	A
	ATOM	437	C	PRO			58.848	20.642	7.824		19.76	A
	ATOM	438	Ō	PRO			58.544	19.700	8.550		16.99	A
	ATOM	439	N	TYR	Α	126	57.947	21.418	7.235		18.98	A
15	ATOM	440	CA	TYR			56.516	21.220	7.435		21.97	A
	ATOM	441	СВ	TYR			55.752	22.448	6.933		25.17	A
	ATOM	442	CG	TYR			56.040	.23.690	7.748		30.98	A
	ATOM	443		TYR			55.438	23.886	8.991		33.95	A
	ATOM	444		TYR			55.721	25.015	9.763		36.60	A
20	ATOM	445	CD2				56.938	24.657	7.292		35.43	A
20	ATOM	446	CE2				57.231	25.792	8.058		37.20	A
	ATOM	447	CZ	TYR			56.618	25.962	9.291		37.40	A
	ATOM	448	ОН	TYR			56.903	27.073	10.052		40.85	A
	ATOM	449	C	TYR			55.990	19.956	6.762	1.00	21.35	A
25	ATOM	450	0	TYR			55.265	19.175	7.383	1.00	20.49	·A
	ATOM	451	N	VAL	Α	127	56.354	19.746	5.501	1.00	18.16	A
	ATOM	452	CA	VAL	Α	:127	55.892	18.562	4.790	1.00	17.58	A
	ATOM	453	CB	VAL	Α	127	56.308	18.596	3.308	1.00	17.45	\mathbf{A}
	ATOM	454	CG1	VAL	Α	127	55.786	17.350	2.600	1.00	17.97	A
30	ATOM	455	CG2	VAL	Α	127	55.751	19.850	2.641	1.00	14.90	A
	MOTA	456	С	VAL	Α	127	56.459	17.306	5.448	1.00	18.39	· A
	ATOM	457	0	VAL	Α	127	55.769	16.298	5.583	1.00	18.14	Ą
	ATOM	458	N	THR	A	128	57.716	17.381	5.869	1.00	17.50	A
	ATOM	459	CA	THR	Α	128	58.375	16.260	6.530		18.54	A
. 35	ATOM	460	CB	THR	Α	128	59.861	16.586	6.805	1.00	18.01	A
	ATOM	461	OG1	THR	Α	128	60.537	16.804	5.559		21.14	A
	ATOM	462	CG2	THR			60.536	15.446	7.545		17.95	A
	ATOM	463	C	THR			57.676	15.941	7.856		19.49	A
	MOTA	464	0	THR			57.438	14.776	8.179		18.76	A
40	ATOM	465	N	ARG			57.345	16.981	8.619		19.60	A
	ATOM	466	CA	ARG			56.673	16.804	9.904		20.12	A
	MOTA	467	CB	ARG			56.534	18.144	10.621		21.33	A
	MOTA	468	CG	ARG			55.948	18.029	12.023		28.02	A
	ATOM	469	CD	ARG			55.721	19.404	12.597		31.25	A
45	ATOM	470	NE	ARG			56.940	20.205	12.560		37.78	A
	MOTA	471	CZ	ARG			56.962	21.524	12.391		40.10	A
	ATOM	472		ARG			55.828	22.197	12.239		40.03	A
	ATOM	473		ARG			58.119	22.170	12.374		44.58	A
	ATOM	474	С	ARG			55.288	16.186	9.729		20.08	A ·
50	ATOM	475	0	ARG	A	129	54.891	15.305	10.496			A
	ATOM	476	N	GLU			54.553	16.654	8.724		18.79 20.10	A A
	ATOM	477	CA	GLU			53.222	16.125	8.454			
_	ATOM	478	CB	GLU			52.638	16.749	7.183 6.708		19.92 27.85	A A
55	MOTA	479	CG	GLU			51.350 50.581	16.087	5.707		29.72	A
55	ATOM	480	CD	GLU				16.933 17.528	4.814		33.46	· A
	ATOM	481		GLU GLU			51.216	16.996	5.807		30.74	A
	ATOM	482	C C	GLU			49.339 53.301	14.615	8.295		19.81	A
	ATOM	483	0	GLU			52.553	13.875	8.935		18.37	A
	ATOM	484	U	GTO	M	130	32.333	13.013	0.900	1.00	-0.57	**

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	ATOM	485		ARĢ A 131		54.219	14.162	7.447	1.00 20.41	· .
	ATOM	486				54.397		7.202	1.00 22.45	P
	MOTA	487				55.442	12.511	6.098	1.00 25.16	P
~	ATOM	488				55.742	11.043	5.840	1.00 28.75	P
5	ATOM	489				56.736	10.837	4.708	1.00 33.75	A
	ATOM	490				57.020	9.415	4.520	1.00 40.07	A
	ATOM	491				57.756	8.915	3.532	1.00 43.07	A
	ATOM	492		1 ARG A 131		58.293	9.721	2.625	1.00 44.91	A
10	MOTA	493		2 ARG A 131		57.955	7.606	3.449	1.00 44.45	A
10	ATOM	494	С	ARG A 131		54.820	11.982	8.466	1.00 23.24	A
	ATOM	495	0	ARG A 131		54.241	10.948	8.804	1.00 23.86	· A
	ATOM	496	N	ASP A 132		55.831	12.497	9.160	1.00 21.99	A
	ATOM	497	CA	ASP A 132		56.318	11.850	10.370	1.00 22.04	A
15	ATOM	498	CB	ASP A 132		57.570	12.564	10.888	1.00 23.72	A
15	ATOM	499	CG	ASP A 132		58.750	12.442	9.932	1.00 27.77	A
	ATOM	500		1 ASP A 132		58.681	11.620	8.989	1.00 27.34	A
	ATOM	501 502		2 ASP A 132		59.753	13.163	10.128	1.00 28.70	A
	ATOM ATOM		С	ASP A 132		55.258	11.772	11.474	1.00 21.69	A
20	ATOM	503 504	O N	ASP A 132 VAL A 133		55.077	10.723	12.092	1.00 22.75	Α
20	ATOM	505	CA	VAL A 133		54.551	12.868	11.725	1.00 19.54	A
	ATOM	506	CB	VAL A 133		53.525	12.843	12.759	1.00 18.52	A
	ATOM	507		VAL A 133		52.908 51.708	14.244	12.990	1.00 19.26	A
	ATOM	508		2 VAL A 133		53.953	14.135	13.918	1.00 18.79	A
25	ATOM	509	C	VAL A 133		52.419	15.180	13.604	1.00 18.80	A
25	ATOM	510	Ö	VAL A 133		52.419	11.854 10.991	12.398	1.00 19.46	A
	ATOM	511	N	MET A 134		51.878	11.957	13.200 11.187	1.00 19.94 1.00 19.15	A
	ATOM	512	CA	MET A 134		50.807	11.052	10.792	1.00 19.15	A
	ATOM	513	CB	MET A 134		50.309	11.381	9.383	1.00 21.25	A
30	ATOM.	514	CG	MET A 134		49.615	12.730	9.302	1.00 17.34	A A
	ATOM	515	SD	MET A 134		48.643		7.798	1.00 20.00	A
	ATOM	516	CE	MET A 134	•	47.033	12.434	8.400	1.00 23.20	A
	ATOM	517	C	MET A 134		51.203	9.582	10.881	1.00 22.43	A
	ATOM	518	0	MET A 134		50.384	8.741	11.249	1.00 23.82	A
35	ATOM	519	N	SER A 135		52.454	9.273	10.556	1.00 23.09	A
	ATOM	520	CA	SER A 135		52.939	7.895	10.615	1.00 26.13	A
	ATOM	521	CB	SER A 135	•	54.356	7.798	.10.039	1.00 26.17	A
	ATOM	522	OG	SER A 135		54.383	8.177	8.673	1.00 31.91	A
	MOTA	523	С	SER A 135		52.957	7.358	12.045	1.00 26.58	A
40	MOTA	524	0	SER A 135		52.926	6.148	12.261	1.00 26.42	A
	ATOM	525	N	ARG A 136		53.014	8.261	13.018	1.00 25.65	Α
	ATOM	526	CA	ARG A 136		53.056	7.870	14.425	1.00 27.47	A
	ATOM	527	CB	ARG A 136		53.823	8.914	15.238	1.00 27.97	A
	ATOM	528	CG	ARG A 136		55.283	9.082	14.857	1.00 32.00	A
45	ATOM	529	CD	ARG A 136		55.904	10.218	15.664	1.00 33.03	A
	ATOM	530	NE	ARG A 136		55.602	10.073	17.084	1.00 36.11	· A
	ATOM	531	CZ	ARG A 136		55.867	10.990	18.007	1.00 39.74	. A
	ATOM	532		ARG A 136		56.449		17.661	1.00 40.55	A
50	ATOM	533		ARG A 136		55.540	10.769	19.276	1.00 36.72	A
50 .	ATOM	534	С	ARG A 136		51.667	7.709	15.036	1.00 26.38	A
	ATOM	535	0	ARG'A 136		51.516	7.121	16.106	1.00 27.06	A
	ATOM	536	N	LEU A 137		50.655	8.235	14.360	1.00 24.77	A
	ATOM	537	CA	LEU A 137		49.294	8.162	14.870	1.00 24.70	A
55	ATOM	538	CB	LEU A 137		48.483	9.363	14.371	1.00 24.52	A
,,	ATOM	539	CG	LEU A 137		49.050	10.760	14.662	1.00 26.67	A
	ATOM	540		LEU A 137		48.075	11.813	14.141	1.00 27.25	A
	ATOM ATOM	541 542		LEU A 137		49.279	10.945	16.155	1.00 27.09	A
	ATOM		С	LEU A 137		48.592	6.868	14.473	1.00 25.20	A
	ATOM	543	0	LEU A 137		48.619	6.469	13.309	1.00 25.99	. А

	ATOM	544	N	ASP	A 138	4	17.971	6.218	15.451	1.00 2	1 80	71
•	ATOM	545	CA	•	A 138		7.239	4.977	15.219	1.00 21		A
	ATOM	546	CB									A
					A 138		18.124	3.761	15.523	1.00 22		Ą
-	ATOM	547	CG		A 138		7.432	2.448	15.201	1.00 24		A
5	MOTA	548		ASP A			16.631	2.423	14.241	1.00 24		A
	MOTA	549	OD2	ASP A		4	7.691	1.443	15.897	1.00 25	5.39	A
	ATOM	550	С	ASP A	138	4	6.031	4.991	16.138	1.00 20	.47	A
	ATOM	551	0	ASP A	138	4	5.967	4.248	17.118	1.00 19	9.06	A
	ATOM	552	N	HIS A	139	4	5.075	5.852	15.810	1.00 18		A
10	ATOM	553	CA	HIS A	139		3.869	6.016	16.606	1.00 18		A.
	ATOM	554	CB	HIS A			4.096	7.157	17.612	1.00 15		A
	ATOM	555	CG	HIS A					18.600			
							2.985	7.332		1.00 15		A
	ATOM	556		HIS A			2.884	6.964	19.900	1.00 13		A
	ATOM	557		HIS A			1.791	7.943	18.280	1.00 14		A
15	ATOM	558		HIS A			1.002	7.944	19.341	1.00 14	.19	. A
	ATOM	559	NE2	HIS A	139	4	1.641	7.356	20.336	1.00 14	.15	A
	ATOM	560	С	HIS A	139	4	2.715	6.330	15.654	1.00 18	.50	· A
	ATOM	561	0	HIS A	139	4	2.879	7.080	14.693	1.00 20	0.80	A
	ATOM	562	N	PRO F	140	4	1.527	5.767	15.913	1.00 18		A
20	ATOM	563	CD	PRO F			1.143	4.984	17.100	1.00 16		A
	ATOM (CA	PRO F			0.367	6.001	15.048	1.00 17		· A
	ATOM	565	CB	PRO F			9.273	5.157		1.00 17		
									15.704			A
	ATOM	566	CG	PRO F			9.643	5.204	17.152	1.00 18		A
	ATOM	567	С	PRO F			9.914	7.441	14.803	1.00 18		A
25	MOTA	568	0	PRO P	140		9.207	7.695	13.831	1.00 19		A
	ATOM	569	N	PHE F		4	0.301	8.381	15.664	1.00 17	.14	Α
	ATOM	570	CA	PHE P	141	3	9.874	9.767	15.477	1.00 16	.42	· A
	ATOM.	571	CB	PHE P	141	3	9.568	10.422	16.836	1.00 14	.60	Α
	ATOM	572	CG	PHE P	141		8.386	9.817	17.556	1.00 15		A
30	ATOM	573	~	PHE F			7.335	9.234	16.842	1.00 14		A
	ATOM	574		PHE A			8.297	9.880	18.942	1.00 13		A
	ATOM	575		PHE P			6.215	8.727	17.502	1.00 16		A
		576		PHE A								
	ATOM						7.178	9.375	19.615	1.00 15		A
	ATOM	577	CZ	PHE P			6.135	8.799	18.893	1.00 16		A
35	MOTA	578	С	PHE P			0.857	10.641	14.694	1.00 16		A
	MOTA	579	0	PHE A			0.799	11.871	14.761	1.00 17		A
	MOTA	580	N	PHE A			1.748	10.011	13.941	1.00 1.5		. A
	ATOM	581	CA	PHE A	142	4	2.727	10.756	13.154	1.00 17	.89	A
	MOTA	582	CB	PHE A	142	4	4.115	10.645	13.793	1.00 17	.57	A
40	ATOM	583	CG	PHE A	142	4	4.240	11.371	15.103	1.00 18	.74	A
	ATOM	584	CD1	PHE A	142	4	4.559	12.726	15.135	1.00 17	.77	A
	MOTA	585	CD2	PHE A	142	4	3.997	10.711	16.304	1.00 18		A
	ATOM	586		PHE A			4.632	13.417	16.347	1.00 15		A
	ATOM	587		PHE A			4.065	11.393	17.522	1.00 17		A
45	ATOM	588		PHE A			4.383					
43			CZ					12.747	17.542	1.00 17		A
	MOTA	589	С	PHE A			2.793	10.231	11.729	1.00 19		A
	MOTA	590	0	PHE A			2.659	9.030	11.504	1.00 20		A
	MOTA	591	N	VAL A			2.978	11.135	10.769	1.00 18		. A
	MOTA	592	CA	VAL A		4	3.102	10.735	9.371	1.00 18	. 52	A
50	ATOM	593	CB	VAL A	143	4	3.294	11.961	8.440	1.00 20	.66	Α
	ATOM	594	CG1	VAL A	143	4	3.843	11.521	7.080	1.00 21	.29	A
	ATOM	595	CG2	VAL A	143	. 4	1.958	12.673	8.252	1.00 22		A
	ATOM	596	С	VAL A			4.342	9.865	9.330	1.00 18		A
	ATOM	597	ō	VAL A			5.355	10.199	9.943	1.00 18		A
55	ATOM	598	N	LYS A			4.259	8.745	8.623	1.00 18		A
55	ATOM			LYS A			5.384	7.824	8.535	1.00 18		
		599	CA									. A
	ATOM	600	CB	LYS A			4.889	6.373	8.608	1.00 22		· A
	ATOM	601	CG	LYS A			6.017	5.340	8.557	1.00 29		A
	ATOM	602	CD	LYS A	144	4	5.491	3.912	8.674	1.00 34	.16	A

	ATOM	603	CE LYS A 144		46.631	2.896	8.577	1.00 37.67	A
	ATOM	604	NZ LYS A 144		46.138	1.484	8.629	1.00 39.02	A
		605	C LYS A 144		46.192	8.002	7.261	1.00 18.53	A
	ATOM					8.314	6.200		A
_	MOTA	606	O 'LYS A 144		45.643			1.00 18.18	
5	MOTA	607	N LEU A 145		47.502	7.816	7.385	1.00 16.79	A
	MOTA	608	CA LEU A 145		48.411	7.900	6.251	1.00 17.45	A
	ATOM	609	CB LEU 145		49.686	8.653	6.641	0.50 18.82	AC1
	ATOM	610	CG LEU 145		50.734	8.902	5.549	0.50 20.23	AC1
	ATOM	611	CD1 LEU 145		51.836	9.799	6.093	0.50 18.83	AC1
10	ATOM	612	CD2 LEU 145		51.317	7.581	5.069	0.50 19.79	AC1
10		613	C LEU A 145		48.739	6.450	5.907	1.00 19.19	A
	ATOM				49.451	5.772	6.659	1.00 17.36	A
	ATOM	614	O LEU A 145				4.782	1.00 17.30	A
	ATOM	615	N TYR A 146		48.215	5.972			
	ATOM	616	CA TYR A 146		48.444	4.593	4.358	1.00 17.57	A
15	ATOM	617	CB TYR A 146		47.288	4.098	3.486	1.00 17.74	Α
	ATOM	618	CG TYR A 146		45.981	3.926	4.214	1.00 17.50	A
	ATOM	619	CD1 TYR A 146		45.099	4.995	4.377	1.00 16.50	A
	ATOM	620	CE1 TYR A 146		43.881	4.827	5.039	1.00 17.10	A
	ATOM	621	CD2 TYR A 146		45.620	2.686	4.735	1.00 18.28	A
20	ATOM	622	CE2 TYR A 146		44.411	2.506	5.399	1.00 19.84	A
20			CZ TYR A 146		43.547	3.576	5.544	1.00 17.53	· A
	ATOM	623			42.342	3.376	6.169	1.00 20.67	_
	MOTA	624			42.342	4.376	3.582	1.00 18.72	A
	MOTA	625	C TYR A 146				3.715	1.00 10.72	A
	MOTA	626	O TYR A 146		50.382	3.338			A
25	MOTA	627	N PHE A 147		50.110	5.350	2.765	1.00 18.09	
	ATOM	628	CA PHE A 147		51.307	5.203	1.952	1.00 17.20	A
	ATOM	629	CB PHE A 147		51.007	4.258	0.783	1.00 16.77	A
	ATOM	630	CG PHE A 147		49.835	4.699	-0.070	1.00 17.75	Α
	ATOM	631	CD1 PHE A 147		49.967	5.752	-0.975	1.00 16.58	A
30	ATOM	632	CD2 PHE A 147		48.595	4.075	0.053	1.00 18.07	A
30		633	CE1 PHE A 147		48.886	6.178	-1.742	1.00 19.62	A
	ATOM		CE2 PHE A 147		47.503	4.492	-0.710	1.00 18.56	Α
	ATOM	634			47.647	5.546	-1.610	1.00 19.27	A
	MOTA	635	CZ PHE A 147			6.533	1.395	1.00 17.13	A
	ATOM	636	C PHE A 147		51.768			1.00 17.13	A
35	MOTA	637	O PHE A 147		51.045	7.528	1.452		A
	MOTA	638	N THR A 148		52.981	6.534	0.854	1.00 17.12	
	ATOM	639	CA THR A 148		53.541	7.718	0.232	1.00 17.96	A
	ATOM	640	CB THR A 148		54.449	8.531	.1.197	1.00 21.51	A
	ATOM	641	OG1 THR A 148		55.605	7.760	1.537	1.00 18.83	A
40	ATOM	642	CG2 THR A 148		53.700	8.897	2.472	1.00 19.60	A
	ATOM	643	C THR A 148		54.386	7.262	-0.946	1.00 20.31	A
	ATOM	644	O THR A 148		54.860	6.124	-0.991	1.00 18.94	Α
		645	N PHE A 149		54.543	8.149	-1.916	1.00 19.16	Α
	ATOM				55.368	7.877	-3.073	1.00 18.01	Α
	MOTA	646			54.748	6.801		1.00 17.23	A
45	ATOM	647	CB PHE A 149				-4.544	1.00 16.88	A
	MOTA	648	CG PHE A 149		53.389	7.144			A
	ATOM	. 649	CD1 PHE A 149		53.262	7.888	-5.712	1.00 18.58	A
	MOTA	650	CD2 PHE A 149		52.235	6.668	-3.927	1.00 17.31	
	ATOM	651	CE1 PHE A 149	•	52.007	8.149	-6.267	1.00 19.26	A
50	MOTA	652	CE2 PHE A 149		50.972	6.923	-4.470	1.00 19.17	A.
	MOTA	653	CZ PHE A 149		50.858	7.663	-5.642	1.00 19.60	A
	ATOM	654	C PHE A 149		55.542	9.205	-3.774	1.00 20.85	A
		655	O PHE A 149		54.934	10.200	-3.376	1.00 19.76	A
	MOTA				56.398	9.241	-4.782	1.00 19.79	A
	ATOM	656			56.636	10.481	-5.497	1.00 24.03	A
55	ATOM	657	CA GLN A 150			11.347	-4.739	1.00 24.45	A
	ATOM	658	CB GLN A 150		57.659		-4.414	1.00 24.43	A
	ATOM	659	CG GLN A 150		58.986	10.645		1.00 20.20	A
	ATOM	660	CD GLN A 150		59.988	11.558	-3.692		
	ATOM	661	OE1 GLN A 150		60.693	12.353	-4.321	1.00 27.05	A

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	ATOM .	662	NE2	GLN	A :	150	60.042	!	11.449	-2.365	1.00	26.47	A
	ATOM	663	С	GLN			57.160)	10.203	-6.885	1.00	23.88	A
	ATOM	664	Ö	GLN			57.673		9.118	-7.158	1.00	24.79	A
	ATOM	665	N	ASP			56.987		11.171	-7.774		25.88	· A
5		666	CA	ASP			57.527		11.047	-9.117		26.49	A
3	ATOM			ASP			56.437			-10.199		24.54	A
	ATOM	667	CB							-10.155		24.95	A
	ATOM	668	CG	ASP			55.544						
	ATOM	669		ASP			56.005		13.379	-9.561		22.44	A
	ATOM	670		ASP			54.369			-10.490		25.72	A
10	ATOM	671	С	ASP			58.515		12.203	-9.220		28.63	A
	ATOM	672	0	ASP	A :	151	58.890	}	12.780	-8.194		27.83	A
	ATOM	673	N	ASP	A :	152	58.934	:	12.560	-10.426		29.21	Α.
	ATOM	674	CA	ASP	A :	152	59.907	,	13.636	-10.562	1.00	31.88	Α
	ATOM	675	СВ	ASP	A :	152	60.325	,	13.792	-12.026	1.00	33.94	A
15	ATOM	676	CG	ASP			61.033	}		-12.557	1.00	38.88	A
13	ATOM	677		ASP			61.817			-11.791	1.00	39.67	A
	ATOM	678		ASP			60.817			-13.738		41.57	A
		679	C	ASP			59.487			-10.013		30.90	A
	ATOM						60.316		15.735	-9.482		31.69	A
	MOTA	680	0	ASP								29.44	A
20	MOTA	681	N	GLU			58.207			-10.107			A
	ATOM	682	CA	GLU			57.767		16.632	-9.646		28.69	
	MOTA	683	CB	GLU			56.984			-10.766		32.90	A
	ATOM	684	CG	GLU			57.451			-12.183		40.57	A
	ATOM	685	CD	GLU	Α	153	56.920)		-12.675		45.78	A
25	ATOM	686	OE1	GLU	Α	153	55.682	?		-12.760		48.91	A
	ATOM	687	OE2	GLU	Α	153	57.736	5	14.747	-12.979		48.95	A
	ATOM	688	С	GLU	Α	153	56.929	•	16.683	-8.372		26.43	A
	ATOM	689	0	GLU	Α	153	56.947	,	17.688	-7.660		25.08	A
	ATOM	690	N	LYS			56.205	5	15.610	-8.069	1.00	22.39	A
30	ATOM	691	CA	LYS			55.318	3	15.631	-6.912	1.00	21.43	A
50	ATOM	692	CB	LYS			53.861		15.628	-7.398	1.00	20.33	A
	MOTA	693	CG	LYS			53.505		16.716	-8.403		21.92	Α
	ATOM	694	·CD	LYS			52.211		16.375	-9.146	1.00	19.70	A
				LYS			51.775			-10.077		20.04	A
25	ATOM	695	CE	LYS			50.631			-10.951		19.97	A
35	ATOM	696	NZ						14.522	-5.881		20.43	A
	ATOM	697	C	LYS			55.458		13.426	-6.173		21.13	A
	MOTA	698	0	LYS			55.949			-4.676		19.69	A
	MOTA	699	N	LEU			54.985		14.832			19.10	A
	ATOM	700	CA	LEU			54.950		13.900	-3.553			A
40 ·	ATOM	701	CB	LEU			55.362		14.588	-2.252		19.65	
	ATOM	702	CG	LEU			56.740		15.234	-2.129		21.20	A
	ATOM	703	CD1	LEU	A	155	56.848		15.918	-0.770		23.42	A
	ATOM	704	CD2	LEU	Α	155	57.816	5	14.174	-2.277		23.08	A
	ATOM	705	С	LEU	Α	155	53.478	3	13.507	-3.427		18.87	A
45	ATOM	706	0	LEU	Α	155	52.600)	14.348	-3.620		18.61	A
	ATOM	707	N	TYR			53.209	9	12.249	-3.091	1.00	15.02	Α
	ATOM	708	CA	TYR			51.834		11.783	-2.934	1.00	16.29	A
	ATOM	709	СВ	TYR			51.470		10.769	-4.029	1.00	14.20	Α
	ATOM	710	CG	TYR			51.603		11.273	-5.449	1.00	17.29	A
50		711		TYR			52.857		11.429	-6.045		16.46	A
30	ATOM						52.978		11.884	-7.360		18.68	A
	ATOM	712		TYR			50.474		11.588	-6.202		16.43	A
	MOTA	713		TYR					12.048	-7.512		16.31	A
	ATOM	714		TYR			50.583			-8.083		18.17	A
	MOTA	715	CZ	TYR			51.835		12.192	•		17.47	A
55	ATOM	716	OH	TYR			51.941		12.651	-9.371			
	MOTA	717	С	TYR			51.657		11.108	-1.572		16.32	. A
	MOTA	718	0	TYR			52.412		10.197	-1.235		16.27	A
	ATOM	719	N	PHE			50.678		11.568	-0.792		15.47	A
	ATOM	720	CA	PHE	A	157	50.385	5	10.966	0.508	1.00	16.66	. A

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	MOTA	721	СВ	PHE	À	157		50.324	12.014	1.629	1.00	16.91	A
•	ATOM	722	CG	PHE	Α	157		51.631	12.708	1.907	1.00	18.96	Ä
	ATOM	723		. PHE				52.821	12.261	1.340	1.00	20.31	A
	ATOM	724	CD2	PHE	Α	157		51.664	13.829	2.732	1.00	21.12	A
5	ATOM	725		PHE				54.025	12.926	1.585	1.00	22.08	А
	ATOM	726	CE2	PHE	A	157		52.865	14.500	2.982	1.00	22.18	A
	MOTA	72 7	CZ	PHE	Ą	157		54.045	14.045	2.405	1.00	21.27	A ·
	MOTA	728	C	PHE	A	157		49.016	10.308	0.404	1.00	16.52	A
	MOTA	729	0	PHE	A	157		48.029	10.979	0.110	1.00	17.32	A
10	ATOM	730	N	GLY	A	158		48.953	9.002	0.644	1.00	15.97	Α
	ATOM	731	CA	GLY	Α	158		47.684	8.299	0.572	.1.00	16.13	A
	MOTA	732	С	GLY	Α	158		47.000	8.383	1.920	1.00	14.94	Α
	MOTA	733	0	GLŸ	Α	158		47.445	7.756	2.879		16.28	·A
	ATOM	734	И	LEU	Α	159		45915	9.145	1.989	1.00	13.50	A
.15	MOTA	735	CA	LEU	A	159		45.191	9.340	3.241	1.00	15.20	A
	ATOM	736	CB	LEU	Α	159		45.031	10.835	3.517	1:00	14.20	· A
	MOTA	737				159		46.270	11.726	3.385	1.00	19.00	A
	MOTA	738	CD1	LEU	Α	159		45.847	13.188	3.477	1.00	17.12	A
	ATOM	739	CD2	LEU	A	159		47.275	11.390	4.471	1.00	14.71	A
20	MOTA	740	С	LEU	Α	159		43.809	8.716	3.232	1.00	15.53	A
	ATOM	741	0	LEU	Α	159		43.232	8.472	2.177		16.05	А
	ATOM	742	N			160		43.268	8.469	4.418		15.86	Α
	ATOM	743	CA			160		41.932	7.917	4.498		19.01	Α
	ATOM	744	CB			160		41.566	7.582	5.949		22.90	. A
25	ATOM	745	OG			160		41.901	8.629	6.833		24.18	. A
	ATOM	746	C			160		40.987	8.968	3.924		20.43	A
	MOTA	747	0			160		41.213	10.173	4.062		19.96	A
	ATOM	748	N			161		39.945	8.508	3.250		19.20	A
	MOTA	749	CA			161		38.975	9.406	2.644		20.37	A
30	MOTA	750	CB			161		38.471	8.785	1.332		20.00	A
	ATOM	751	CG			161		37.314	9.502	0.666		20.72	A
	ATOM	752		TYR				37.222	10.895	0.682		18.22	A
	ATOM	753		TYR				36.180	11.557	0.029		22.24	A
0.5	ATOM	754		TYR				36.333	8.784	-0.020		20.53	. A
35	ATOM	755		TYR				35.287	9.436	-0.678		24.24	A
	ATOM	756	CZ			161		35.218	10.822	-0.648		22.32	A
	ATOM	757	OH	TYR				34.194	11.471	-1.298		23.03	A
	ATOM	758	С	TYR				37.812	9.681	3.598		20.14	, A
40	ATOM	759	0	TYR				36.959	8.819	3.810		19.53	A ·
40	MOTA	760	N	ALA				37.791	10.880	4.178		19.92	A
	MOTA	761	CA	ALA				36.721 37.187	11.271	5.099		21.07 19.60	A
	ATOM ATOM	762 763	CB C	ALA ALA				35.542	12.419 11.712	6.002 4.238		22.07	A
	ATOM	763 764	0	ALA				35.342	12.875	3.860		20.66	A A
45		765	N	LYS				34.653	10.769	3.945		23.27	
75	ATOM ATOM	766	CA.	LYS				33.503	11.017	3.080		27.12	A A
	ATOM	767	CB	LYS				32.663	9.741	2.963		29.68	A
	ATOM	768	CG	LYS				33.455	8.524	2.515		37.67	A
	ATOM	769	CD	LYS				32.556	7.310	2.313		42.24	A
50	ATOM	770	CE	LYS				33.373	6.034	2.185		44.48	A
30	ATOM	771	NZ	LYS				34.143	5.735	3.430		44.88	A ·
	ATOM	772	C	LYS				32.581	12.186	3.411		25.78	. A
	ATOM	773	0	LYS				32.103	12.863	2.506		26.53	A
	ATOM	774	И	ASN				32.327	12.441	4.689		24.57	A
55	ATOM	775	CA	ASN				31.420	13.522	5.033		23.77	A _.
	ATOM	776	CB	ASN				30.610	13.129	6.265		25.02	A.
	ATOM	777	CG	ASN				29.537	12.101	5.932		27.54	A
	MOTA	778		ASN				28.772	12.281	4.983		28.79	A.
	ATOM	779		ASN				29.475	11.024	6.704		27.13	A
					- •				,,	3.752	2.00	2	

	ATOM	780	С	ASN	Α	164	31.999	14.931	5.169	1.00	24.43	A
	ATOM	781	0	ASN	Α	164	31.306	15.856	5.589		23.98	· A
	ATOM	782	N	GLY	Α	165	33.262	15.097	4.795		21.56	A
	ATOM	783	CA	GLY	A.	165	33.873	16.414	4.836	1.00	24.39	Α
5	ATOM	784	C .	GLY	Α	165	34.191	17.043	6.181	1.00	23.62	A
	ATOM	785	0	GLY	Α	165	34.380	16.352	7.177		23.26	A
	ATOM	786	N	GLU	A	166	34.234	18.373	6.186	1.00	23.22	Α
	ATOM	787	CA	GLU			34.563	19.176	7.362	1.00	24.54	A
	ATOM	788	CB	GLU			35.055	20.558	6.913		25.04	A
10	ATOM	789	CG	GLU			36.419	20.569	6.229		26.48	A
	ATOM	790	CD	GLU			36.699	21.889	5.517		30.02	Α
	ATOM	791		GLU			36.081	22,906	5.889		29.33	A
	ATOM	792	OE2	GLU	А	166	37.544	21.916	4.596	1.00	30.48	A
	ATOM	793	С	GLU			33.436	19.372	8.369		24.44	А
15	ATOM	794	0	GLU	Α	166	32.279	19.541	8.001		22.76	A
	ATOM	795	N	LEU			33.791	19.370	9.649		22.95	A
	ATOM	796	CA	LEU			32.813	19.581	10.707		22.26	Α
	ATOM	797	CB	LEU			33.497	19.481	12.073		22.32	Α
	ATOM	798	CG	LEU			32.706	19.923	13.306		22.04	A
20	ATOM	799		LEU			31.454	19.074	13.463		19.66	Α
	ATOM	800		LEU			33.597	19.805	14.537		21.17	Α
	ATOM	801	C	LEU			32.193	20.971	10.529		23.49	A
	MOTA	802	ō	LEU			31.047	21.209	10.907		23.56	A
	ATOM	803	N	LEU			32.960	21.887	9.948		24.25	А
25	ATOM	804	CA	LEU			32.473	23.245	9.722		26.64	A
23	ATOM	805	CB	LEU			33.560	24.099	9.066	1.00	25.62	A
	ATOM	806	CG	LEU			33.198	25.546	8.707		27.34	Α
	ATOM	807		LEU			32.718	26.296	9.946		26.42	A
	ATOM	808		LEU			34.418	26.238	8.119		26.74	Α
30	ATOM	809	C	LEU			31.234	23.218	8.829		27.13	Α
50	ATOM	810	0.	LEU			30.297	23.989	9.030		26.01	Α
	ATOM	811	N	LYS			31.233	22.320	7.848		26.41	A
	ATOM	812	CA	LYS			30.106	22.210	6.934		27.70	Α
	ATOM	813	СВ	LYS			30.324	21.064	5.945		30.49	Α
35	ATOM	814	CG	LYS			29.151	20.854	4.993		32.47	Α
33	ATOM	815	CD	LYS			29.407	19.728	3.998		35.98	Α
	ATOM	816	CE	LYS			29.462	18.372	4.683		38.53	A
	ATOM	817	NZ	LYS			29.622	17.263	3.702		41.00	· A
	ATOM	818	C	LYS			28.801	21.985	7.682		28.12	Α
40	ATOM	819	ō	LYS			27.785	22.608	7.371		28.08	Α
40	ATOM	820	N	TYR			28.826	21.094	8.668		26.53	A
	ATOM	821	CA	TYR			27.624	20.791	9.434		26.95	Α
	ATOM	822	CB	TYR			27.810	19.476	10.193		25.03	Α
•	ATOM	823	CG	TYR			27.898	18.300	9.251	1.00	26.65	A
45	ATOM	824		TYR			26.745	17.661	8.790		28.27	A
7.5	ATOM	825		TYR			26.814	16.642	7.839		26.85	A
	ATOM	826		TYR			29.127	17.884	8.742		27.83	A
	ATOM	827		TYR			29.209	16.869	7.792	1.00	27.19	A
	ATOM	828	CZ	TYR			28.049	16.254	7.343		30.02	A
50	ATOM	829	ОН	TYR			28.130	15.268	6.382		29.23	A
50	ATOM .	830	C	TYR			27.229	21.918	10.376		27.59	A
	ATOM	831	Ö	TYR			26.045	22.122	10.642		29.25	A
	ATOM	832	N	ILE			28.208	22.660	10.882		28.16	A
	ATOM	833	CA.	ILE			27.883	23.770	11.763		29.03	A
55	ATOM	834	CB	ILE			29.151	24.435	12.337		27.51	A
-	ATOM	835		ILE			28.773	25.705	13.084		27.97	A
	ATOM	836		ILE			29.872	23.458	13.272		26.70	A
	MOTA	837		ILE			31.163	23.996	13.856		24.07	A
	ATOM	838	C	ILE			27.094	24.796	10.944		31.41	A
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	ATOM	839	0	ILE	Α	171		26.088	25.335	11.407	1.00	31.69	A
	ATOM	840	N	ARG			•	27.546	25.047	9.719	1.00	33.21	· A
	ATOM	841	CA	ARG	A	172		26.874	26.000	8.844	1.00	36.54	A
	ATOM	842	СВ	ARG				27.734	26.314	7.616		37.73	A ·
5	ATOM	843	CG	ARG				29.057	27.011	7.912		41.65	A
,		844	CD	ARG				29.708	27.492	6.616		45.29	A
	ATOM			ARG					28.070	6.812		48.51	A
	MOTA	845	NE					31.037		7.658		51.53	A
	ATOM	846	CZ	ARG				31.314	29.059				
	ATOM	847		ARG				30.355	29.593	8.406		53.75	A
10	ATOM	848		ARG				32.553	29.526	7.748		51.21	A
	ATOM	849	С	ARG				25.528	25.459	8.378		37.67	A
	ATOM	850	0	ARG	Α	172		24.550	26.200	8.288		39.09	A
	ATOM .	851	N	LYS	Α	173		25.481	24.163	8.092	1.00	38.44	A
	ATOM	852	CA	LYS	Α	173		24.259	23.528	7.619	1.00	39.25	Α
15	ATOM	853	CB .	LYS	А	173		24.523	22.061	7.272	1.00	41.89	A
~~	ATOM	854	CG	LYS				23.279	21.298	6.830	1.00	45.52	A·
	ATOM	855	CD	LYS				23.557	19.808	6.653		49.60	Α
	ATOM	856	CE	LYS				24.477	19.530	5.469		52.63	A
		857	NZ	LYS				23.855	19.894	4.160		54.61	A
	ATOM							23.033	23.608	8.595		39.30	A
20	ATOM	858	C	LYS						8.201		39.62	A
	ATOM	859	0	LYS			•	21.981	23.960			37.96	A
	ATOM	860	N	ILE				23.320	23.282	9.863			A
	ATOM	861	CA	ILE				22.229	23.314	10.833		37.36	
	ATOM	862	CB	ILE			-	22.159	21.998	11.652		37.44	A
25	MOTA	863	CG2	ILE	А	174	•	22.058	20.802	10.709		38.37	A
	ATOM	864	CG1	ILE	Α	174		23.397	21.850	12.532		37.25	A
	ATOM	865	CD1	ILE	Α	174		23.355	20.620	13.418		36.85	A
	MOTA	866	С	ILE	A	174		22.259	24.492	11.801	1.00	36.71	A
	MOTA	867	0	ILE	Α	174		21.448	24.556	12.724		38.05	A
30	ATOM	868	N	GLY	Α	175		23.185	25.423	11.592	1.00	35.48	A
50	ATOM	869	CA	GLY				23.265	26.585	12.462	1.00	35.29	A
	ATOM	870	C	GLY				24.053	26.360	13.737	1.00	35.06	A
	ATOM	871	Ö	GLY				25.066	27.019	13.970	1.00	37.46	A
	ATOM	872	N	SER				23.581	25.441	14.571		33.94	A
26		873	CA	SER				24.253	25.113	15.822		32.84	A
35	ATOM							23.938	26.155	16.901		33.54	A
	ATOM	874	CB	SER				22.599	26.056	17.347		34.86	A
	ATOM	875	OG	SER					23.731	16.276		32.34	A
	MOTA	876	С	SER				23.796	23.731	15.884		32.82	A
	ATOM	877	0	SER				22.726		17.103		29.39	A
40	MOTA	878	N	PHE				24.609	23.085			27.20	A
	MOTA	879	CA	PHE				24.313	21.743	17.597			A
	MOTA	880	CB	PHE				25.621	20.989	17.865		26.39	
	MOTA	881	CG	PHE				26.372	20.585	16.622		26.18	A
	MOTA ·	882	CD1	PHE	Α	177		26.210	21.277	15.426		25.30	A
45	ATOM	883	CD2	PHE	Α	177		27.266	19.516			26.05	A
	ATOM	884	CE1	PHE	Α	177		26.923	20.912	14.290		26.59	Α
	ATOM	885	CE2	PHE	A	177		27.986	19.143	15.532		26.06	A
	ATOM	886	CZ	PHE				27.815	19.841	14.343	1.00	25.42	A
	ATOM	887	C.	PHE				23.500	21.752	18.884	1.00	27.00	A
50	ATOM	888	Ö	PHE				23.704	22.610	19.747	1.00	26.48	A
50	ATOM	889	N	ASP				22.578	20.802	19.022	1.00	26.70	A
				ASP				21.816	20.729	20.260		26.35	A
	ATOM	890	CA	ASP				20.621	19.773	20.142		29.90	A
	ATOM	891	CB					21.020	18.372	19.720		32.28	A
	MOTA	892	CG	ASP						20.014		35.21	A
55	ATOM	893		ASP				22.157	17.949	19.105		34.79	A
	ATOM	894		ASP				20.179	17.683			25.03	A
	MOTA	895	C	ASP				22.810	20.228	21.311			
	MOTA	896	0	ASP				23:974	19.968	20.992		21.24	A
	ATOM	897	N	GLU	A	179		22.361	20.083	22.552	1.00	23.60	A

	ATOM	898	CA	GLU A	179	23.247	19.644	23.619	1.00 25.18	A
	ATOM	899	CB	GLU A	179	22.542	19.770	24.971	1.00 27.60	Α
	ATOM	900	CG	GLU A	179	23.324	19.176	26.130	1.00 32.58	A
	ATOM	901	CD	GLU A	179	22.997	19.845	27.449	1.00 35.82	A
5	ATOM	902	OE1	GLU A	179	21.825	20.224	27.645	1.00 35.95	· A
	ATOM	903	OE2	GLU A	179	23.912	19.984	28.291	1.00 38.19	Α
	ATOM	904	С	GLU A		23.808	18.235	23.450	1.00 24.08	, A
	ATOM	905	0	GLU A	179	24.977	17.989	23.756	1.00 22.79	A
	ATOM	906	N	THR A	180	22.983	17.316	22.961	1.00 23.36	A
10	ATOM	907	CA	THR A	180	23.412	15.935	22.761	1.00 22.15	A
20	ATOM	908	СВ	THR A		22.224	15.054	22.320	1.00 23.77	A
	ATOM	909	-	THR A		21.222	15.075	23.341	1.00 26.37	A
	ATOM	910		THR A		22.670	13.616	22.088	1.00 22.66	Α
	ATOM	911	C	THR A		24.533	15.830	21.724	1.00 22.01	A
15	ATOM	912	ō	THR A		25.533	15.141	21.944	1.00 19.87	Α
13	ATOM	913	N	CYS A		24.365	16.511	20.596	1.00 21.21	A
	ATOM	914	CA	CYS A		25.372	16.480	19.541	1.00 22.22	A
	ATOM	915	CB	CYS A		24.800	17.065	18.250	1.00 24.62	Α
	ATOM	916	SG	CYS A		23,435	16.080	17.560	1.00 29.50	Α
20	ATOM	917	c	CYS A		26.633	17.232	19.954	1.00 23.07	A
20	ATOM	918	ō	CYS A		27.746	16.827	19.608	1.00 23.95	Α
	ATOM	919	N	THR A		26.463	18.325	20.695	1.00 22.76	A
	ATOM	920	CA	THR A		27.606	19.103	21.161	1.00 21.49	A
	ATOM	921	СВ	THR A		27.167	20.346	21.978	1.00 21.37	· A
25.	ATOM	922		THR A		26.459	21.262	21.134	1.00 22.50	A
23	ATOM	923		THR A		28.379	21.046	22.565	1.00 18.36	A
	ATOM	924	С	THR A	182	28.454	18.215	22.071	1.00 21.48	A
	ATOM	925	0	THR A		29.669	18.090	21.894	1.00 19.95	A
	ATOM	926	N	ARG A	183	27.798	17.602	23.050	1.00 18.97	A
30	ATOM	927	CA	ARG A	183	28.468	16.723	23.996	1.00 19.39	A
	ATOM	928	CB	ARG	183	27.455	16.140	24.984	0.50 19.46	AC1
	ATOM	929	CG	ARG	183	28.030	15.062	25.887	0.50 18.77	AC1
	ATOM	930	CD	ARG	183	27.021	14.571	26.925	0.50 21.19	AC1
	ATOM	931	NE	ARG	183	26.605	15.642	27.824	0.50 19.46	AC1
35	ATOM	932	CZ	ARG	183	25.496	16.362	27.679	0.50 20.45	AC1
	ATOM	933	NH1	ARG	183	24.672	16.123	26.666	0.50 19.81	AC1
	ATOM	934	NH2	ARG	183	25.224	17.338	28.539	0.50 17.11	AC1
	ATOM	935	С	ARG A	183	29.206	15.577	23.302	1.00 20.02	A A
	MOTA	936	0	ARG A		30.383	15.333	23.573	1.00 19.97	A
40	MOTA	937	N	PHE A		28.520	14.871	22.409	1.00 19.24 1.00 18.04	A
	ATOM	938	CA	PHE A		29.144	13.746	21.722	1.00 21.05	A
	ATOM	939	CB	PHE A		28.158	13.078	20.764 20.098	1.00 22.67	. A
	ATOM	940	CG	PHE A		28.719	11.857	20.036	1.00 22.07	A
	ATOM	941		PHE A		28.717	10.630		1.00 19.97	A
45	MOTA	942		PHE A		29.317	11.949	18.850	1.00 23.57	A
	MOTA	943		PHE A		29.308	9.510	20.176 18.263	1.00 23.33	A
	ATOM	944		PHE A		29.915	10.833	18.928	1.00 24.11	A
	MOTA	945	CZ	PHE A		29.910	9.613 14.127	20.941	1.00 22.37	A
	ATOM	946	C	PHE A		30.403	13.531	21.130	1.00 17.33	Α .
50	ATOM	947	0	PHE A		31.461		20.056	1.00 15.73	A
	MOTA	948	N	TYR A		30.292	15.110 15.519	19.265	1.00 15.73	A
	MOTA	949	CA	TYR A		31.443 30.992	16.413	18.111	1.00 17.33	A
	ATOM	950	CB	TYR A		30.364	15.584	17.015	1.00 17.33	A
	ATOM	951	CG	TYR A		31.159	14.809	16.168	1.00 16.53	A
55	ATOM	952		TYR A		30.590	13.952	15.232	1.00 18.12	A
	MOTA	953		TYR A		28.976	15.484	16.892	1.00 18.18	A
	ATOM	954		TYR A		28.398	14.623	15.956	1.00 18.90	A
	ATOM	955 956		TYR A		29.211	13.861	15.133	1.00 18.41	A
	ATOM	956	CZ	IIK	. 100	27.211	-3.501			

								,		
	ATOM -	957	OH	TYR A	185	28.650	12.995	14.218	1.00 20.48	A
	ATOM	958	C	TYR A		32.544	16.172	20.083	1.00 15.79	A
	ATOM	959	ŏ	TYR F		33.720	16.015	19.766	1.00 17.69	A
							16.887			
~	ATOM	960	N	THR A		32.176		21.142	1.00 15.68	A
5	ATOM	961	CA	THR A		33.184	17.504	21.997	1.00 16.03	A
	ATOM	962	CB	THR F	186	32.559	18.403	23.094	1.00 16.62	A
	ATOM	963	OG1	THR A	186	31.866	19.503	22.481	1.00 14.79	A
	ATOM	964	CG2	THR A	186	33.656	18.953	24.019	1.00 14.68	A
	ATOM	965	С	THR A	186	33.954	16.375	22.680	1.00 15.59	A
10	ATOM	966	ō	THR A		35.176	16.443	22.823	1.00 13.77	A
10	ATOM	967	N	ALA A		33.234	15.333	23.097	1.00 14.06	A
								23.757		
	ATOM	968.	CA		187	33.869	14.196		1.00 14.74	A
	ATOM	969	CB	ALA A		32.810	13.195	24.224	1.00 14.32	A
	MOTA	970	С	ALA A	187	34.875	13.509	22.821	1.00 14.41	A
15	MOTA	971	0	ALA A	187	35.972	13.136	23.247	1.00 15.61	A
	MOTA	972	N	GLU A	188	34.516	13.340	21.549	1.00 14.01	A
	ATOM	973	CA	GLU A		35.443	12.704	20.615	1.00 13.50	A
	ATOM	974	CB	GLU F		34.782	12.449	19.251	1.00 12.85	A
	ATOM	975	CG	GLU F		33.622	11.454	19.282	1.00 12.71	A
20	MOTA	976	CD	GLU A		33.464	10.685	17.979	1.00 15.01	A
	MOTA	977	OE1	GLU F	188	33.687	11.275	16.899	1.00 13.21	A
	ATOM	978	OE2	GLU F	188	33.110	9.484	18.031	1.00 17.69	A
	ATOM	979	С	GLU A	188	36.682	13.582	20.436	1.00 13.34	A
	MOTA	980	0	GLU A	188	37.803	13.085	20.408	1.00 14.69	Α
25	ATOM	981	N	ILE A		36.486	14.893	20.326	1.00 13.52	A
23	ATOM	982	CA	ILE A		37.627	15.787	20.159	1.00 13.35	A
						37.169	17.247	19.939	1.00 13.95	A
	ATOM		CB	ILE F						A
	ATOM	984		ILE F		38.381	18.165	19.822	1.00 12.47	
	ATOM	985		ILE A		36.302	17.332	18.671	1.00 13.44	A
30	MOTA	986	CD1	ILE F	189	35.588	18.664	18.491	1.00 14.29	A
	ATOM	987	С	ILE A	189	38.530	15.702	21.394	1.00 14.63	A
	ATOM	988	0	ILE A	189	39.753	15.595	.21.271	1.00 12.97	A
	ATOM	989	N	VAL A		37.927	15.751	22.582	1.00 14.35	A
	ATOM	990	CA	VAL A		38.684	15.655	23.832	1.00 13.22	A
35	ATOM	991	CB	VAL A		37.743	15.690	25.061	1.00 14.28	Ά
33						38.509	15.267	26.326	1.00 15.08	A
	ATOM	992		VAL A					1.00 13.00	A
	MOTA	993		VAL A		37.160	17.082	25.233		
	ATOM	994	С	VAL A		39.468	14.338	23.859	1.00 14.61	A
	ATOM	995	0	VAL A		40.634		24.250	1.00 13.72	A
40	MOTA	996	N	SER A	191	38.825	13.254	23.432	1.00 15.26	A
	ATOM	997	CA	SER A	191	39.478	11.943	23.421	1.00 16.81	A
	ATOM	998	CB	SER	191	38.470	10.857	23.041	0.50 16.14	AC1
	ATOM	999	OG	SER	191	39.018	9.569	23.238	0.50 16.94	AC1
	ATOM	1000	C	SER A		40.649	11.928	22.441	1.00 16.58	A
15			_			41.697	11.335	22.713		A
45	ATOM	1001	0	SER A					1.00 15.26	
	MOTA	1002	N	ALA A		40.468	12.586	21.300		A
	ATOM	1003	CA	ALA A		41.518	12.645	20.292	1.00 14.37	A
	MOTA	1004	CB	ALA A	192	40.989	13.296	19.016	1.00 14.43	A
	ATOM	1005	С	ALA A	192	42.695	13.440	20.845	1.00 16.46	A
50	ATOM	1006	0	ALA A	192	43.851	13.038	20.697	1.00 17.96	A
	ATOM	1007	N	LEU A		42.401	14.563	21.496	1.00 15.02	A
	ATOM	1008	CA	LEU A		43.459	15.392	22.067	1.00 15.42	A
				LEU A		42.884	16.712	22.600	1.00 12.88	A
	ATOM	1009	CB						1.00 12.00	A
	MOTA	1010	CG	LEU F		42.445	17.721	21.525		
55	MOTA	1011		LEU F		41.869	18.979	22.190	1.00 13.97	A
	ATOM	1012	CD2	LEU A		43.642	18.088	20.655	1.00 14.58	A
	ATOM	1013	С	LEU F	193	44.211	14.659	23.174	1.00 14.49	A
	ATOM	1014	0	LEU A	193	45.427	14.813	23.310	1.00 16.56	A
	ATOM	1015	N	GLU F		43.500	13.870	23.975	1.00 13.96	A
				_						

	ATOM	1016	CA	GLU A	194	44.179	13.123	25.032	1.00 14.08	Α
	ATOM	1017	CB	GLU A	194	43.190	12.295	25.857	1.00 14.65	A
	ATOM	1018	CG	GLU A	194	43.882	11.301	26.789	1.00 17.09	A
	MOTA	1019	CD	GLU A	194	42.924	10.592	27.730	1.00 19.59	A
5	ATOM	1020	OE1	GLU A		41.809	10.237	27.295	1.00 19.25	A
	ATOM	1021		GLU A		43.302	10.380	28.906	1.00 20.20	A
	ATOM	1022	C	GLU A		45.208	12.199	24.386	1.00 13.57	Â
	ATOM	1023	ō	GLU A		46.337	12.093	24.847	1.00 14.23	A
	ATOM	1024	N	TYR A		44.822	11.544	23.301	1.00 14.25	A
10	ATOM	1025	CA	TYR A		45.743	10.642	22.618	1.00 14.89	A
10	ATOM	1026	CB	TYR A		45.030	9.910	21.488	1.00 10.38	
	ATOM	1027	CG	TYR A		45.956	9.058	20.649	1.00 17.29	A
	ATOM	1027		TYR A		46.347	7.788	21.077		A
		1028							1.00 17.96	A
15	MOTA		CE1			47.203	6.996	20.304	1.00 19.77	A
15	ATOM .	1030	CD2			46.445	9.524	19.428	1.00 16.67	. A
	ATOM	1031	CE2			47.299	8.744	18.650	1.00 18.51	A
	ATOM	1032	CZ	TYR A		47.671	7.481	19.094	1.00 20.24	A
	ATOM	1033	OH	TYR A		48.506	6.705	18.325	1.00 21.89	Α
	ATOM	1034	С	TYR A		46.917	11.419	22.035	1.00 16.98	A
20	MOTA	1035	0	TYR A		48.081	11.047	22.203	1.00 14.61	A
	MOTA	1036	N	LEU A		46.599	12.507	21.347	1.00 16.30	A
	MOTA	1037	CA	LEU A		47.619	13.328	20.720	1.00 18.15	A
	ATOM	1038	CB	LEU A		46.969	14.502	19.982	1.00 18.59	A
	ATOM	1039	CG	LEU A		47.834	15.203	18.935	1.00 22.51	A
25	MOTA	1040		LEU A		48.222	14.206	17.841	1.00 20.94	A
	MOTA	1041	CD2	LEU A	196		16.375	18.338	1.00 22.98	A
	MOTA	1042	С	LEU A	196	48.592	13.844	21.763	1.00 17.75	Α
	MOTA	1043	0	LEU A	196	49.801	13.644	21.649	1.00 18.33	A
	MOTA	1044	N	HIS A	197	48.064	14.495	22.792	1.00 17.12	A
30	MOTA	1045	CA	HIS A	197	48.913	15.042	23.842	1.00 18.47	A
	ATOM	1046	CB	HIS A	197	48.069	15.866	24.817	1.00 15.90	A
	ATOM	1047	CG	HIS A	197	47:571	17.152	24.231	1.00 19.15	A
	ATOM	1048	CD2	HIS A	197	47.830	17.745	23.038	1.00 18.22	A
	ATOM	1049	ND1	HIS A	197	46.704	17.992	24.897	1.00 17.47	A
35	MOTA	1050	CE1	HIS A	197	46.450	19.047	24.139	1.00 19.74	A -
	ATOM	1051	NE2	HIS A	197	47.119	18.921	23.007	1.00 15.69	A
	ATOM	1052	С	HIS A	197	49.696	13.958	24.572	1.00 19.40	A
	ATOM	1053	0	HIS A	197	50.823	14.192	25.021	1.00 19.42	A
	ATOM	1054	N	GLY A	198	49.106	12.770	24.679	1.00 18.59	A
40	ATOM	1055	CA	GLY A	198	49.793	11.675	25.339	1.00 19.60	. A
	ATOM	1056	С	GLY A	198	51.075	11.307	24.612	1.00 21.86	Α
	ATOM	1057	0	GLY A	198	51.963	10.682	25.186	1.00 23.09	A
	ATOM	1058	N	LYS A		51.174	11.687	23.341	1.00 22.81	A
	ATOM	1059	CA	LYS A	199	52.368	11.401	22.549	1.00 24.43	Α
45	ATOM	1060	CB	LYS A		51.990	10.905	21.154	1.00 26.00	A
	ATOM	1061	CG	LYS A		51.378	9.520	21.133	1.00 30.98	A
	ATOM	1062	CD	LYS A		51.291	9.002	19.708	1.00 36.85	A
	ATOM	1063	CE	LYS A		50.832	7.559	19.682	1.00 40.37	A
	ATOM	1064	NZ	LYS A		51.646	6.691	20.581	1.00 43.48	A
50	ATOM	1065	C	LYS A		53.253	12.631	22.414	1.00 23.88	A
-	ATOM	1066	0	LYS A		54.144	12.669	21.568	1.00 24.97	A
	ATOM	1067	N	GLY A		52.997	13.638	23.243	1.00 24.00	A
	ATOM	1068	CA	GLY A		53.790	14.853	23.203	1.00 22.12	A
	ATOM	1069	C	GLY A		53.665	15.632	21.907	1.00 22.12	A
55	ATOM	1070	Ö	GLY A		54.632	16.231	21.439	1.00 22.14	A
J.J	ATOM	1071	N	ILE A		52.475	15.630	21.320	1.00 20.00	A
	ATOM	1071	CA	ILE A		52.252	16.355	20.080	1.00 20.00	A
				ILE A			15.414	18.955	1.00 18.93	A
	ATOM	1073	CB	ILE A		51.784 51.414		17.716	1.00 19.70	A
	ATOM	1074	UG2	TTT A	2 U I	51.414	16.226	71.170	1.00 20.12	A

	ATOM	i075	CG1	ILE A	201	5	2.880	14.395	18.636	1.00	20.03	Α
	ATOM	1076	CD1	ILE	201		2.408	13.258	17.745		22.75	A
	ATOM	1077	С	ILE A	201		1.193	17.425	20.270		19.87	A
	ATOM	1078	0	ILE A	201		0.121	17.161	20.817		20.08	A
5	ATOM	1079	N	ILE A			1.508	18.633	19.815		19.94	. A
•	ATOM	1080	CA	ILE A			0.601	19.772	19.891		20.45	A
	ATOM	1081	СВ	ILE A			1.352	21.040	20.356		22.21	A
	ATOM	1082		ILE A			0.381	22.220	20.470		22.67	A
	ATOM	1083	CG1				2.033	20.775	21.700		24.19	
10	ATOM	1084	CD1				2.033	21.920	22.169		25.39	A A
10		1084	CDI	ILE A							20.71	
	ATOM			ILE A			0.105	19.999	18.464			A
	ATOM	1086	0				0.910	20.067	17.538		19.48	A
	ATOM	1087	N	HIS A			8.795	20.108	18.270		18.65	A
1.5	ATOM	1088	CA	HIS A			8.280	20.319	16.919		18.02	A
15	ATOM	1089	CB	HIS A			6.775	20.057	16.874		16.31	A
	ATOM	1090	CG	HIS A			6.199	20.136	15.495		18.36	A
	MOTA	1091		HIS A			6.043	21.186	14.655		16.42	A
	MOTA	1092		HIS A			5.759	19.026	14.806		19.50	A
	MOTA	1093		HIS A			5.359	19.389	13.600		17.64	A
20	MOTA-	1094	NE2	HIS A			5.522	20.694	13.483		20.87	A
	MOTA	1095	С	HIS A		4	8.589	21.738	16.405		18.92	A
	MOTA	1096	0	HIS A			9.073	21.906	15.282		16.21	A
	MOTA	1097	N	ARG A	204	4	8.301	22.744	17.232	1.00	18.60	A
	MOTA	1098	CA	ARG A	204	4	8.552	24.157	16.914		19.81	A
25	MOTA	1099	CB	ARG A	204	4	9.998	24.365	16.458	1.00	21.61	A
	MOTA	1100	CG	ARG A	204	5	1.024	24.137	17.550		23.82	A
	MOTA	1101	CD	ARG A	204	5	2.323	24.870	17.252	1.00	27.62	A
	ATOM	1102	NE	ARG A	. 204	5	2.932	24.449	15.994	1.00	29.43	A
	ATOM .	1103	CZ	ARG A	204	5	4.125	24.861	15.572	1.00	33.10	A
30	MOTA	1104	NH1	ARG A	204	5	4.835	25.706	16.311		32.12	A
	ATOM	1105	NH2	ARG A	204	5	4.614	24.426	14.418	1.00	30.25	A
	MOTA	1106	С	ARG A	204	4	7.624	24.830	15.905	1.00	20.03	Α
	ATOM	1107	0	ARG A	204.	4	7.711	26.038	15.698	1.00	20.88	A
	ATOM	1108	· N	ASP A	205	4	6.755	24.071	15.255	1.00	18.96	Α
35	ATOM	1109	CA	ASP A	205	4	5.828	24.692	14.325	1.00	17.90	А
•	ATOM	1110	CB	ASP A	205	4	6.418	24.741	12.914	1.00	18.95	Α
	ATOM	1111	CG	ASP A	205	4	5.655	25.688	12.008	1.00	20.36	A
	ATOM	1112	OD1	ASP A	205	4	4.939	26.560	12.545	1.00	20.35	A
	ATOM-	1113	OD2	ASP A	205	4	5.772	25.573	10.771	1.00	22.49	A
40	MOTA	1114	С	ASP A	205	4	4.500	23.956	14.328	1.00	19.60	Α
	ATOM	1115	0	ASP A	205	4	3.876	23.751	13.287	1.00	21.53	A
	ATOM	1116	N	LEU A	206	4	4.063	23.569	15.521	1.00	18.53	A
	ATOM	1117	CA	LEU A	206	. 4	2.813	22.851	15.667	1.00	19.18	A
	ATOM	1118	СВ	LEU A	206	4	2.693	22.295	17.087	1.00	18.94	Α
45	ATOM	1119	CG	LEU A	206	4	1.511	21.358	17.346	1.00	23.10	A
	ATOM	1120		LEU A			1.615	20.142	16.436		23.01	A
	ATOM	1121		LEU A			1.504	20.933	18.808		22.97	Α
	ATOM	1122	С	LEU A			1.639	23.772	15.361	1.00	19.05	Α
	ATOM	1123,		LEU A			1.556	24.880	15.886	1.00	19.25	A
50	ATOM	1124	N	LYS A			0.740	23.307	14.500		17.54	' A
	MOTA	1125	CA	LYS A			9.564	24.081	14.110		18.60	Α
	ATOM	1126	СВ	LYS A			9.980	25.248	13.196	1.00	18.98	Α
	ATOM	1127	CG	LYS A			0.786	24.817	11.982		18.20	A
	ATOM	1128	CD	LYS A			1.246	26.000	11.139		21.42	A
55	ATOM	1129	CE	LYS A			2.223	25.537	10.062		23.21	A
	ATOM	1130	NZ	LYS A			2.561	26.604	9.084		29.61	A
	ATOM	1131	C	LYS A			8.566	23.181	13.388		18.18	A
	ATOM	1132	ō	LYS A			8.921	22.100	12.915		18.11	A
	ATOM	1133	N	PRO A			7.298	23.614	13.293		20.26	A
						_					_	

	MOTA	1134	CD	PRO A	208		36.713	24.833	13.882	1.00	18.79		A
•	MOTA	1135	CA	PRO A	208		36.272	22.814	12.616	1.00	19.67		A
	ATOM	1136	CB	PRO A	208		35.063	23.742	12.608	1.00	19.45		Α
	MOTA	1137	CG	PRO A	208		35.231	24.509	13.891	1.00	21.81		A
5	MOTA	1138	С	PRO F	208		36.674	22.372	11.209	1.00	21.04		A
	MOTA	1139	0	PRO A			36.264	21.307	10.751	1.00	21.19		A
	MOTA	1140	N	GLU A	209		37.474	23.188	10.528	1.00	21.69		A
	ATOM	1141	CA	GLU A			37.928	22.872	9.170	1.00	22.64		A
	MOTA	1142	CB	GLU	209		38.644	24.084	8.558	0.50	23.65		AC1
10	MOTA	1143	CĢ.	GLU	209		39.253	23.825	7.185		27.24		AC1
	MOTA	1144	CD	GLU	209		40.155	24.958	6.716		29.40		AC1
	MOTA	1145	OE1		209		39.660	26.094	6.553		29.68		AC1
	MOTA	1146	OE2		209		41.363	24.711	6.511		30.07		AC1
	MOTA	1147	С	GLU F			38.879	21.668	9.159		22.28		A
15	ATOM	1148	0	GLU F			38.955	20.933	8.170		21.36		A
	ATOM	1149	N	ASN A			39.600	21.490	10.263		19.90		A
	ATOM	1150	CA	ASN A			40.574	20.412	10.436		19.44		A
	ATOM	1151	CB	ASN A			41.744	20.912	11.287		20.07		A
	MOTA	1152	CG	ASN A			42.746	21.698	10.479		25.77		A
20	MOTA	1153		ASN A			43.571	22.427	11.029		26.73		A
	ATOM	1154		ASN A			42.687	21.548	9.158		25.15		A
	MOTA	1155	С	ASN A			40.005	19.151	11.078		18.63		A
	ATOM	1156	0	ASN A			40.712	18.154	11.234		18.29		A
25	ATOM	1157	N	ILE A			38.739	19.202 18.058	11.469		16.31		A A
25	MOTA	1158	CA	ILE A			38.090 37.336	18.488	12.085 13.354		15.49		A
	ATOM	1159 1160	CB CG2				36.582	17.311	13.354		14.59		A
	ATOM ATOM	1161		ILE A			38.342	19.046	14.365		15.91		A
	ATOM	1162		ILE A			37.720	19.669	15.590		15.98		Α
30	ATOM	1163	CDI	ILE A			37.131	17.485	11.059		17.26		A
50	ATOM	1164	Ó	ILE A			35.995	17.947	10.926		18.16		A
	MOTA	1165	N	LEU A			37.599	16.486	10.317		15.97		A
	ATOM	1166	CA	LEU A			36.784	15.875	9.274		17.08		A
	ATOM	1167	CB	LEU F			37.685	15.249	8.202		17.78		A
35	ATOM	1168	CG	LEU A			38.785	16.157	7.640		18.92		Α
	ATOM	1169		LEU A			39.476	15.450	6.485	1.00	22.09		A
	ATOM	1170		LEU A		•	38.188	17.482	7.166	1.00	19.91		Α
	ATOM	1171	С	LEU A			35.843	14.825	9.837	1.00	18.35		A
	ATOM	1172	0	LEU A	212		35.957	14.433	11.002	1.00	19.39	-	Α
40	MOTA	1173	N	LEU A	213		34.915	14.368	9.000		17.84		Α.
	ATOM	1174	CA	LEU A	213		33.942	13.362	9.403	.1.00			A
	ATOM	1175	CB	LEU A	213		32.556	14.004	9.487	1.00	20.84		A
	MOTA	1176	CG	LEU A	213		32.396	15.059	10.583		20.31		A
	MOTA	1177		LEU A			31.124	15.837	10.367		22.75		A
45	ATOM	1178	CD2	LEU A				14.378	11.940		23.93		A
	MOTA	1179	С	LEU A			33.914	12.187	8.426		20.98		Α
	MOTA	1180	0	LEU A			33.743	12.379	7.218		19.55		A
	MOTA	1181	N	ASN A			34.088	10.970	8.935		20.44		A
	MOTA	1182	CA	ASN A			34.055	9.814	8.049		23.77		A
50	ATOM	1183	СВ	ASN A			34.745	8.596	8.674		25.30		A
	ATOM	1184	CG	ASN A		•	34.077	8.127	9.948		32.04		A
	ATOM	1185		ASN A			32.908	8.422	10.206		34.43		A
	MOTA	1186		ASN A			34.818	7.369	10.752		33.85		A n
	ATOM	1187	C	ASN A			32.618	9.466	7.693		24.07		A n
55	ATOM	1188	0	ASN A			31.672	10.113	8.150		19.94		A a
	ATOM	1189	N	GLU A			32.459 31.138	8.433	6.879 6.445		25.77 28.69		A A
	ATOM	1190	CA	GLU A				8.003 6.796	5.513		31.98		A
	MOTA	1191	CB	GLU A			31.275	6.334	4.896		40.22		A
	MOTA	1192	CG	GLU A	213		29.970	0.334	4.090	1.00	40.22		Λ.

_	MOTA	1193	CD	GLU :	A 215		30.182	5.312	3.795	1.00 44.27	А
•	ATOM	1194		L GLU			30.817				
	ATOM	·1195		GLU Z			29.716				
	ATOM	1196			A 215						A
. 5	ATOM					•	30.188	7.673		1.00 28.41	A
,		1197			A 215		28.971	7.769		1.00 28.52	A
	MOTA	1198			A 216		30.737	7.287	8.752	1.00 26.77	A
	MOTA	1199	CA	ASP A	A 216		29.914	6.953	9.917	1.00 27.28	A
	MOTA	1200		ASP A	A 216		30.538	5.795	10.696	1.00 31.27	A
	ATOM	1201	CG	ASP A	A 216		30.390	4.466	9.979	1.00 37.61	A
10	ATOM	1202		ASP A			29.274	4.170	9.499	1.00 37.01	A
	ATOM	1203		ASP A			31.382	3.710	9.902		
	ATOM	1204	C	ASP A			29.697			1.00 41.84	A
	ATOM	1205						8.135	10.862	1.00 26.37	Α
			0	ASP A			29.136	7.984	11.950	1.00 25.73	A
1.5	ATOM	1206	N	MET A			30.156	9.306	10.441	1.00 23.02	Α
15	ATOM	1207	CA	MET A			30.015	10.527	11.218	1.00 21.83	A
	ATOM	1208	CB	MET A	1 217		28.537	10.789	11.517	1.00 23.24	A
	ATOM	1209	CG	MET A	217		27.742	11.186	10.274	1.00 22.98	A
	ATOM	1210	SD	MET A			28.464	12.616	9.430	1.00 27.57	A
	ATOM	1211	CE				27.679	13.974	10.332		
20	ATOM	1212	C	MET P						1.00 26.68	. A.
20	ATOM	1213					30.844	10.618	12.502	1.00 21.51	A
			0	MET A			30.474	11.323	13.440	1.00 18.62	А
	ATOM	1214	N	HIS A			, 31.957	9.892	12.544	1.00 20.10	Α
	ATOM	1215	CA	HIS A			32.873	9.964	13.678	1.00 19.86	. A
	ATOM	1216	CB	HIS A	218		33.482	8.594	13.977	1.00 20.21	A
25	MOTA	1217	CG	HIS A	218		32.551	7.667	14.698	1.00 22.40	A
	ATOM	1218	CD2	HIS A	218		31.910	6.547	14.287	1.00 21.27	A
	ATOM	1219		HIS A			32.177	7.863	16.011	1.00 19.59	A
	ATOM	1220		HIS A			31.348	6.902	16.379		
	ATOM	1221		HIS A						1.00 21.88	A
30	ATOM	1222					31.168	6.091	15.351	1.00 22.08	A
50			C	HIS A			33.947	10.921	13.172	1.00 19.10	A
	ATOM	1223	0	HIS A			34:170	11.004	11.965	1.00 20.31	Α
	MOTA	1224	N	ILE A			34.617	11.638	14.067	1.00 17.21	A
	MOTA	1225	CA	ILE A			35.628	12.586	13.618	1.00 15.26	A
	ATOM	1226	CB	ILE A	219		35.987	13.614	14.716	1.00 15.38	A
35	ATOM	1227	CG2	ILE A	219		34.722	14.305	15.221		A
	ATOM	1228		ILE A			36.734	12.919	15.864	1.00 14.46	A
	ATOM	1229		ILE A			37.279	13.885	16.911	1.00 13.74	
	ATOM	1230	C	ILE A			36.929	11.944			A
	ATOM	1231	Ö	ILE A					13.161	1.00 16.21	A
40	ATOM	1232					37.238	10.799	13.500	1.00 15.88	· A
70			N	GLN A			37.677	12.711	12.378	1.00 15.62	A
	ATOM	1233	CA	GLN A			38.980	12.316	11.876	1.00 17.84	Α
	MOTA	1234	CB	GLN A			38.872	11.595	10.525	1.00 20.00	A
	ATOM	1235	CG	GLN A	220		38.463	10.129	10.659	1.00 26.97	A
	ATOM	1236	CD	GLN A	220		38.648	9.343	9.372	1.00 29.95	A
45	ATOM	1237	OE1	GLN A	220		37.968	9.590	8.373	1.00 33.12	A
	ATOM	1238		GLN A			39.578	8.393	9.389	1.00 30.47	A
	ATOM	1239	С	GLN A			39.757	13.610	11.735		
	ATOM	1240		GLN A			39.609			1.00 17.00	A
	ATOM	1241						14.339	10.751	1.00 18.27	A
50			N	ILE A			40.566	13.906	12.746	1.00 14.34	A
50	MOTA	1242		ILE A			41.361	15.120	12.753	1.00 14.46	A
	ATOM	1243		ILE A			41.867	15.416	14.175	1.00 12.30	A
	ATOM	1244		ILE A			42.764	16.656	14.167	1.00 14.78	A
	MOTA	1245	CG1	ILE A	221		40.660	15.613	15.102	1.00 13.92	A
	MOTA	1246		ILE A			41.003	15.901	16.543	1.00 15.06	A
55	ATOM	1247		ILE A			42.536	14.996	11.783	1.00 15.44	
	ATOM	1248		ILE A			43.106				. A
	ATOM	1249		THR A				13.915	11.613	1.00 13.93	A
							42.877	16.101	11.127	1.00 15.36	A
	ATOM	1250		THR A			43.980	16.098	10.174	1.00 17.52	A
	ATOM	1251	CB	THR A	222		43.470	15.836	8.750	1.00 19.92	A

	ATOM	1252	OG1	THR F	222		44.587	15.637	7.875	1.00 18.78	A
	MOTA	1253	CĠ2	THR P	222		42.630	17.018	8.257	1.00 18.16	
	ATOM	1254	С	THR A	222		44.735	17.428	10.192	1.00 19.60	
	ATOM	1255	0	THR A	222		44.509	18.257	11.084	1.00 18.59	
5	MOTA	1256	N	ASP A	223		45.630	17.610	9.216	1.00 18.69	
	ATOM	1257	CA	ASP A			46.440	18.825	9.069	1.00 20.12	
	ATOM	1258	СВ	ASP A			45.532	20.065	9.108	1.00 23.51	
	ATOM	1259	CG	ASP A			46.248	21.335	8.670	1.00 27.09	
	ATOM	1260		ASP A			47.283	21.227	7.975	1.00 26.28	
10	ATOM	1261		ASP A			45.765	22.438	9.009	1.00 26.15	
10	ATOM	1262	C	ASP A			47.516	18.913	10.150	1.00 21.73	
	ATOM	1263	ō	ASP A			47.439	19.751	11.055	1.00 21.75	
	ATOM	1264	N	PHE A		•	48.535	18.063	10.027	1.00 22.70	
	ATOM	1265	CA	PHE A			49.611	17.988	11.009	1.00 20.73	
15	ATOM	1266	CB	PHE A			49.805	16.527	11.424	1.00 20.11	
13		1267		PHE A							
	ATOM	1267	CG				48.682	15.991	12.263	1.00 21.41	
	ATOM			PHE A			48.598	16.312	13.614	1.00 23.05	
	ATOM	1269		PHE A			47.681	15.212	11.693	1.00 22.27	A
20	ATOM	1270		PHE A			47.528	15.868	14.389	1.00 23.30	A
20	ATOM	1271		PHE A			46.606	14.763	12.457	1.00 21.11	
	ATOM	1272	CZ	PHE A			46.530	15.093	13.807	1.00 22.02	
	MOTA	1273	С	PHE A			50.957	18.583	10.619	1.00 20.45	
	MOTA	1274	0	PHE A			51.905	18.547	11.407	1.00 20.73	
	ATOM	1275	. N	GLY A			51.049	19.125	9.412	1.00 22.02	A
25	MOTA	1276	CA	GLY A			52.301	19.713	8.981	1.00 22.66	
	MOTA	1277	С	GLY A			52.742	20.822	9.920	1.00 24.99	
	MOTA	1278	0	GLY A			53.939	21.041	10.122	1.00 24.52	A
	MOTA	1279	N	THR A			51.779	21.524	10.508	1.00 23.50	A
	MOTA	1280	CA	THR A			52.106	22.613	11.416	1.00 25.16	
30	MOTA	1281	CB	THR A			51.199	23.829	11.160	1.00 24.76	
	MOTA	1282	OG1	THR A			49.831	23.410	11.113	1.00, 22.68	A
	MOTA	1283	CG2	THR A	226		51.571	24.490	9.834	1.00 25.00	
	MOTA	1284	С	THR A			52.046	22.233	12.894	1.00 25.79	
	MOTA	1285	0	THR A	226	·	52.019		,13.768	1.00 24.54	A
35	MOTA	1286	N	ALA A			52.037	20.935	13.173	1.00 24.97	A
	MOTA	1287	CA	ALA A	227		52.004	20.475	14.550	1.00 25.49	
	MOTA	1288	CB	ALA A			51.659	18.993	14.607	1.00 22.85	Α.
	MOTA	1289	С	ALA A			53.384	20.715	15.149	1.00 27.70	A
	MOTA	1290	0	ALA A			54.331	21.047	14.435	1.00 26.60	A
40	ATOM	1291	N	LYS A			53.491	20.558	16.461	1.00 28.53	
	ATOM	1292	CA	LYS A			54.760	20.745	17.149	1.00 32.12	A
	MOTA	1293	CB	LYS A			54.699	21.974	18.054	1.00 33.81	A
	ATOM	1294	CG	LYS A	228		56.007	22.294	18.765	1.00 41.23	A
	ATOM	1295	CD	LYS A	228		57.082	22.725	17.768	1.00 47.57	A
45	MOTA	1296	CE	LYS A	228		58.401	23.056	18.462	1.00 49.82	A
	MOTA	1297	NZ	LYS A	228		59.459	23.425	17.480	1.00 51.49	A
•	ATOM	1298	С	LYS A	228		55.019	19.504	17.985	1.00 33.25	Α
	ATOM	1299	0	LYS A	228		54.190	19.129	18.815	1.00 33.70	A
	MOTA	1300	N	VAL A	229		56.159	18.860	17.756	1.00 33.64	A
50	MOTA	1301	CA	VAL A			56.516	17.661	18.501	1.00 34.66	A
	MOTA	1302	CB	VAL A	229		57.248	16.646	17.609	1.00 33.50	A
	ATOM	1303	CG1	VAL A	229		57.619	15.419	18.415	1.00 32.34	A
	ATOM	1304	CG2	VAL A			56.370	16.264	16.436	1.00 34.25	A
	ATOM	1305	С	VAL A			57.420	18.035	19.668	1.00 37.57	A
55	ATOM	1306	0	VAL A			58.581	18.392	19.474	1.00 35.91	A
	ATOM	1307	N	LEU A	230		56.877	17.948	20.878	1.00 40.57	A
	ATOM	1308	CA	LEU A			57.615	18.289	22.088	1.00 46.10	A
	MOTA	1309	CB	LEU A			56.654	18.417	23.270	1.00 44.71	A
	ATOM	1310	CG	LEU A	230		55.627	19.545	23.207	1.00 44.50	A

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	MOTA	1311		LEU A		54.673	19.430	24.383		A
	ATOM	1312	CD2	LEU A		56.340	20.885	23.214	1.00 44.81	A
	ATOM	1313	С	LEU A	230	58.695	17.279	22.440	1.00 50.42	A
	ATOM	1314	0	LEU A	230	58.603	16.104	22.089	1.00 51.64	A
5	ATOM	1315	N	SER A		59.717	17.756	23.145	1.00 55.81	A
. •	ATOM	1316	CA	SER A			16.914		1.00 61.14	
							•			A
	ATOM	1317	CB	SER A		62.077	17.200	22.750	1.00 61.27	A
	ATOM	1318	OG	SER A		62.444	18.568	22.823	1.00 62.85	A
	ATOM	1319	C	SER A	231		17.126	25.071	1.00 64.65	A
10	MOTA	1320	0	SER A	231	61.392	16.164	25.794	1.00 65.70	A
	ATOM	1321	N	PRO A	232	61.081	18.387	25.549	1.00 67.54	A
	ATOM	1322	CD	PRO A	232	60.854	19.651	24.823	1.00 68.60	A
	ATOM	1323	CA	PRO F		61.358	18.655	26.966	1.00 68.74	A
	ATOM	1324	СВ	PRO F		61.109	20.158	27.086	1.00 68.83	A
15		1325	CG	PRO F		61.505	20.666	25.737	1.00 68.96	A
15	MOTA									
	ATOM	1326	С	PRO F		60.460	17.846	27.899	1.00 69.17	A
	MOTA	1327	0	PRO F		59.335	17.494	27.541	1.00 69.94	A
	ATOM	1328	N	ALA A	237	`57.424	23.198	27.637	1.00 80.06	A
	ATOM	1329	CA	ALA A	237	56.783	23.047	26.335	1.00 79.29	Α
20	ATOM	1330	CB	ALA A	237	55.275	22.907	26.512	1.00 78.64	A
	ATOM	1331	С	ALA A	237	57.092	24.239	25.433	1.00 79.07	A
	ATOM	1332	ŏ	ALA A		56.250	25.113	25.249	1.00 79.47	A
	ATOM	`1333	N	ALA A		58.297	24.280	24.871	1.00 78.57	A
				ALA A		58.683	25.383	23.992	1.00 78.50	A
	MOTA	1334	CA						1.00 78.50	
25	ATOM	1335	CB	ALA A		60.186	25.347	23.728		A
	MOTA	1336	С	ALA A		57.920	25.327	22.673	1.00 78.15	A
	ATOM	1337	0	ALA A	238	57.243	24.341	22.375	1.00 77.96	A
	ATOM	1338	N	ALA A	239	58.027	26.393	21.887	1.00 77.28	A
	ATOM	1339	CA	ALA A	239	57.338	26.452	20.603	1.00 76.27	A
30	ATOM	1340	CB .	ALA A	239	55.849	26.489	20.827	1.00 76.61	A
	ATOM	1341	C	ALA A		57.766	27.667	19.793	1.00 75.38	A
	ATOM	1342	ō	ALA A		58.955	27.955	19.700	1.00 75.89	A
		1343	N	ASN F		56.781·	28.357	19.214	1.00 73.95	A
	ATOM						29.553	18.389	1.00 73.93	A
	ATOM	1344	CA	ASN A						A
35	MOTA	1345	СВ	ASN A		58.151	30.400	18.874	1.00 71.47	
	MOTA	1346	CG	ASN A		59.459	30.055	18.174	1.00 72.06	A
	MOTA	1347	OD1	ASN A	240	59.575	30.149	16.943	1.00 72.03	A
	MOTA	1348	ND2	ASN A	240	60.470	29.665	18.964	1.00 71.91	A
	ATOM	1349	С	ASN A	240	57.188	29.178	16.928	1.00 69.41	A
40	ATOM	1350	0	ASN A	240	57.480	28.024	16.624	1.00 70.09	A
	ATOM	1351	N	ALA A		57.055	30.165	16.038	1.00 66.62	Α
`	ATOM	1352	CA	ALA A		57.246	30.013	14.585	1.00 63.94	A
	ATOM	1353	C	ALA A		55.952	30.080	13.772	1.00 60.63	Α
		1354	0	ALA A		55.840	30.880	12.845	1.00 61.29	A
4 ~	ATOM		-						1.00 65.23	
45	MOTA	1355	CB	ALA A						
	MOTA	1356	И	PHE A		54.984	29.236	14.113	1.00 56.72	A
	ATOM	1357	CA	PHE P		53.712	29.196	13.394	1.00 52.53	A
	MOTA	1358	CB	PHE F		53.419	27.767	12.923	1.00 49.14	A
	ATOM	1359	CG	PHE P	242	52.040	27.590	12.354	1.00 47.38	A
50	ATOM	1360	CD1	PHE P	242	51.731	28.067	11.085	1.00 47.69	A
	ATOM	1361		PHE F		51.038	26.975	13.102	1.00 45.45	A
	ATOM	1362		PHE P		50.445	27.937	10.565	1.00 46.75	A
		1363		PHE F		49.751	26.840	12.594	1.00 45.41	A
	MOTA					49.453	27.323	11.322	1.00 46.55	A
	ATOM	1364	CZ	PHE .						
55	MOTA	1365	С	PHE F		52.534	29.688	14.229	1.00 50.08	A
	ATOM	1366	0	PHE F		52.502	29.505	15.444	1.00 49.86	A
	MOTA	1367	N	VAL A		51.566	30.305	13.557	1.00 47.67	A
	ATOM	1368	CA	VAL F	243	50.355	30.809	14.200	1.00 46.21	A
	ATOM	1369	CB	VAL A	243	50.340	32.352	14.258	1.00 47.36	A

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	ATOM	1370	CG1	VAL A 243	3.	49.012	32.844	14.825	1.00 47.54	A
	ATOM	1371	CG2	VAL A 243	3	51.497	32.842	15.109	1.00 48.50	A
	ATOM	1372		VAL A 24:		49.150	30.342	13.389	1.00 44.12	A
		1372		VAL A 24		48.956	30.765	12.247	1.00 44.46	A
_	ATOM			GLY A 24		48.348	29.467	13.985	1.00 40.48	A
5	ATOM	1374		GLY A 24		47.176	28.941	13.306	1.00 37.65	A
	ATOM	1375					29.960	12.964	1.00 35.39	A
	MOTA	1376		GLY A 24		46.101		13.065	1.00 35.92	A
	ATOM	1377	0	GLY A 24		46.313	31.168			A
	MOTA	1378	N	THR A 24		44.936	29.463	12.560	1.00 33.30	A
10	ATOM	1379	CA	THR A 24		43.813	30.312	12.184	1.00 30.20	
	MOTA	1380	CB	THR A 24	5	42.593	29.450	11.829	1.00 32.00	A
	ATOM	1381	OG1	THR A 24	5	42.952	28.573	10.755	1.00 32.81	A
	ATOM	1382	CG2	THR A 24	5	41.419	30.319	11.390	1.00 28.34	A
	ATOM	1383	C	THR A 24	5	43.476	31.296	13.296	1.00 27.96	A
1.5		1384	Ö	THR A 24		43.212	30.907	14.434	1.00 25.46	A
15	ATOM			ALA A 24		43.486	32.576	12.938	1.00 25.22	Α
	MOTA	1385	N	ALA A 24		43.247	33.675		1.00 23.27	A
	MOTA	1386	CA	ALA A 24	· ·	42.956	34.955	13.082	1.00 22.94	A
	MOTA	1387	CB	ALA A 24				-14.934	1.00 21.27	A
	MOTA	1388	С	ALA A 24		42.178	33.705	16.114	1.00 20.93	A
20	ATOM	1389	0	ALA A 24		42.431		14.536	1.00 19.67	A
	MOTA	1390	N	GLN A 24		40.988	33.047		1.00 10.07	A
	ATOM	1391	CA	GLN A 24		39.911	32.886	15.504	0.50 21.89	AC1
	MOTA	1392	CB	GLN 24	7	38.608	32.535	14.779		AC1
	ATOM	1393	CG	GLN 24	7	38.522	33.076	13.355	0.50 26.18	
25	ATOM	1394	CD	GLN 24	7	37.220	33.794	13.064	0.50 27.30	AC1
23	ATOM	1395	OE1	GLN 24	7	36.172	33.447	13.605	0.50 30.13	AC1
	ATOM	1396	NE2			37.278	34.792	12.189	0.50 28.70	AC1
	ATOM	1397	C	GLN A 24		40.181	31.849	16.595	1.00 19.43	A
		1398	o	GLN A 24		39.546	31.883	17.648	1.00 18.93	A
	MOTA			TYR A 24		41.132	30.948	16.359	1.00 18.60	A
30	ATOM	1399	N	TYR A 24		41.441	29.896	17.329	1.00 19.20	A
	MOTA	1400	CA			41.333	28.529	16.642	1.00 17.53	A
	MOTA	1401	CB	TYR A 24		40.013	28.362	15.927	1.00 19.32	A
	MOTA	1402	CG	TYR A 24			28.010	16.625	1.00 17.69	A
•	MOTA	1403		TYR A 24		38.859	27.976	15.990	1.00 18.18	A
35	ATOM	1404	CE1	TYR A 24		37.617		14.569	1.00 16.87	` A.
	ATOM	1405	CD2			39.897	28.664	13.924	1.00 19.17	A
	MOTA	1406	CE2	TYR A 24		38.665	28.635		1.00 19.46	A
	MOTA	1407	CZ	TYR A 24	48	37.527	28.295	14.643	1.00 13.40	A
	MOTA	1408	OH	TYR A 24	48	36.299	28.311	14.023		A
40	ATOM	1409	С	TYR A 2	48	42.810	30.039	17.993	1.00 20.42	A
10	ATOM	1410	0	TYR A 2	48	43.208	29.191	18.792	1.00 19.19	
	ATOM	1411	N	VAL A 2		43.523	31.114	17.673	1.00 20.20	A
	ATOM	1412	CA	VAL A 2		44.841	31.343	18.251	1.00 20.91	A
	ATOM	1413	СВ	VAL A 2		45.542	32.532	17.570	1.00 21.18	A
45		1414		VAL A 2		46.821	32.896	18.317	1.00 22.45	A
45	MOTA			VAL A 2		45.862	32.170	16.139	1.00 24.01	A
	ATOM	1415		VAL A 2	10	44.764	31.606		1.00 21.52	A
	ATOM	1416		VAL A 2		43.915	32.368	20.216	1.00 22.72	A
	ATOM	1417	0			45.654	30.965		1.00 20.70	A
	MOTA	1418	N	SER A 2	50	45.697			1.00 21.65	A
50	MOTA	1419	CA	SER A 2	50				1.00 22.02	A
	MOTA	1420	CB	SER A 2		46.370			1.00 22.12	A
	MOTA	1421	OG	SER A 2		47.692		_	1.00 22.13	A
	MOTA	1422	С	SER A 2		46.476			1.00 22.13	A
	MOTA	1423	0	SER A 2		47.332	32.828		1.00 22.77	A
55	MOTA	1424		PRO A 2		46.180				A
-	ATOM	1425		PRO A 2		45.163				
	MOTA	1426		PRO A 2		46.893				A
	MOTA	1427		PRO A 2		46.233				A
	ATOM	1428		PRO A 2		45.726		25.676	1.00 22.55	A
	AIOM	1470								

	ATOM	1429	С	PRO A	251	41	8.414	34.115	23.907	1.00	22.15	А
	ATOM	1430	0	PRO A			9.143	35.047	23.563		22.62	. A
	ATOM	1431	N	GLU A	-		8.901	32.966	24.367		20.69	
	ATOM	1432	CA				0.347	32.772	24.500		21.40	A
5	ATOM	1433	СВ	GLU A			0.673	31.382	25.071		20.59	
•	ATOM	1434	CG	GLU A			9.993	30.232				A
	ATOM	1435	CD	GLU A			-		24.352		21.91	A
							3.691	29.822	25.014		21.51	A
	ATOM	1436		L GLU A			7.989	30.707	25.550		21.46	A
10	ATOM	1437		GLU A			3.367	28.613	24.993		20.23	A
10	ATOM	1438	C	GLU A			1.071	32.970	23.167		22.99	A
	ATOM	1439	0	GLU A			2.191	33.480	23.136		23.17	A
	ATOM	1440	N	LEU A			0.441	32.576	22.064		23.00	A
	MOTA	1441	CA	LEU A			L.068	32.753	20.758		25.62	Α.
	ATOM	1442	СВ	LEU A			277	32.029	19.669	1.00	26.75	A
15	MOTA	1443	ÇG	LEU A		50	0.743	30.620	19.296	1.00	31.87	Α
	ATOM	1444	CD1	LEU A	253	50	0.433	29.651	20.422	1.00	31.81	Α
	MOTA	1445	CD2	LEU A	253	50	0.044	30.179	18.015	1.00	31.86	A
	MOTA	1446	Ć	LEU A	253	51	1.201	34.228	20.371	1.00	26.94	A
	MOTA	1447	0	LEU A	253	. 52	2.107	34.601	19.626	1.00	27.09	A
20	MOTA	1448	N	LEU A	254	50	.297	35.059	20.877		25.83	A
	MOTA	1449	CA	LEU A	254	50	.297	36.485	20.564		27.26	· A
	ATOM	1450	CB	LEU A	254		3.858	37.006	20.564		25.84	A
	ATOM	1451	CG	LEU A	254	47	7.882	36.290	19.621		24.69	· A
	MOTA	1452		LEU A			5.459	36.724	19.932		23.64	. A
25	ATOM	1453		LEU A			3.236	36.597	18.177		24.24	A
	ATOM	1454	C	LEU A			.134	37.314	21.537		30.62	A
	ATOM	1455	ō	LEU A			. 633	38.383	21.187		32.35	A
	ATOM	1456	N	THR A			292	36.821	22.758		32.47	A
	ATOM	1457	CA	THR A			2.056	37.547	23.759		36.70	A
30	ATOM	1458	CB	THR A			.368	37.478	25.127		34.51	
50	ATOM	1459	OG1				.188	36.106	25.494			A
	ATOM	1460	CG2								35.49	A
	MOTA	1461	CGZ	THR A			0.013	38.166	25.077		33.40	A
	ATOM	1461					477	37.035	23.910		40.09	A
35			0	THR A			.430	37.793	23.772		43.69	A
33	MOTA	1463	N	GLU A			617	35.747	24.189		44.77	A
	ATOM	1464	CA	GLU A			.932	35.144	24.382		49.15	A
	ATOM	1465	CB	GLU A			.866	34.143	25.534		51.24	A
	ATOM	1466	CG	GLU A			.514	34.786	26.862		56.03	A
40	ATOM	1467	CD	GLU A			.053	33.780	27.893		58.83	A
40	MOTA	1468	OE1				.766	32.776	28.107		62.13	A
	ATOM	1469	OE2				.979	33.996	28.494		60.34	A
	ATOM	1470	С	GLU A			.475	34.456	23.137		50.09	A
	ATOM	1471	0	GLU A			.616	33.995	23.127		50.42	A
	ATOM	1472	N	LYS A			. 658	34.389	22.090		51.21	A
45	MOTA	1473	CA	LYS A			.064	33.746	20.845	1.00	51.22	A
	ATOM	1474	CB	LYS A			.244	34.502	20.227	1.00	53.28	A
	ATOM	1475	CG	LYS A		56	.558	34.125	18.790	1.00	55.19	A
	ATOM	1476	CD	LYS A	257	57	.709	34.961	18.253	1.00	57.52	A
	ATOM	1477	CE	LYS A	257	57	.952	34.694	16.777	1.00	58.52	A
50	ATOM	1478	NZ	LYS A	257	58	.290	33.268	16.515	1.00	60.88	A
	ATOM	1479	С	LYS A	257	55	.467	32.302	21.138	1.00	50.74	Α
	ATOM	1480	0	LYS A	257	56	.432	31.790	20.577	1.00	52.26	A
	ATOM	1481	N	SER A	258		.721	31.654	22.027		48.07	A
	ATOM	1482	CA	SER A			.999	30.273	22.402		46.87	A
55	ATOM	1483	CB	SER A			.590	30.229	23.812		48.88	A
	ATOM	1484	OG	SER A			.741	30.892	24.734		53.14	A
	ATOM	1485	С	SER A			.735	29.415	22.342			A
	ATOM	1486	ō	SER A			.617	29.932	22.417		44.17	A
	ATOM	1487	N	ALA A			.917	28.105	22.204		38.30	A
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	ATOM	1488	CA	ALA	Α	259		52.793	27.180	22.127	1.00 34.73	A
	MOTA	1489	CB	ALA	Α	259	•	52.551	26.779	20.684	1.00 34.16	· A
	MOTA	1490	С	ALA	Α	259		53.042	25.940	22.977	1.00 32.34	A
	MOTA	1491	0	ALA	Α	259		54.172	25.459	23.086	1.00 31.81	A
5	MOTA	1492	N	CYS	Α	260		51.975	25.428	23.579	1.00 28.58	A
	MOTA	1493	CA	CYS	Α	260		52.056	24.244	24.425	1.00 26.27	A
	MOTA	1494	CB	CYS	Α	260		52.183	24.654	25.892	1.00 26.53	A
	MOTA	1495	SG	CYS	A	260		50.846	25.739	26.469	1.00 32.91	A
	ATOM	1496	С	CYS	Α	260		50.786	23.435	24.224	1.00 22.83	A
10	MOTA	1497	0	CYS	A	260		49.892	23.856	23.495	1.00 22.14	A
	ATOM	1498	N	LYS				50.706	22.277	24.868	1.00 20.02	A
	MOTA	1499	CA	LYS	A	261		49.526	21.434	24.744	1.00 20.65	A
	MOTA	1500	CB	LYS				49.619	20.243	25.696	1.00 23.28	A
	MOTA	1501	CG	LYS				50.716	19.253	25.347	100 27.44	A
15	MOTA	1502	CD	LYS	Α	261		50.732	18.117	26.350	1.00 29.98	A
	MOTA	1503	CE	LYS			•	51.922	17.203	26.134	1.00 32.34	A
	MOTA	1504	NZ	LYS				51.940	16.121	27.153	1.00 33.28	A
	MOTA	1505	С	LYS				48.268	22.229	25.062	1.00 19.20	A
	MOTA	1506	0	LYS				47.253	22.092	24.387	1.00 18.08	A
20	ATOM	1507	N	SER				48.358	23.068	26.089	1.00 16.92	A
	MOTA	1508	CA	SER				47.235	23.883	26.534	1.00 18.13	A
	MOTA	1509	СВ	SER				47.644	24.698	27.770	1.00 18.27	A
	MOTA	1510	OG	SER				46.517	25.258	28.421	1.00 22.53	A
	MOTA	1511	C-	SER				46.736	24.811	25.424	1.00 16.77	A A
25	MOTA	1512	0	SER				45.591	25.254	25.450	1.00 15.69 1.00 16.44	A
	MOTA	1513	N	SER				47.595	25.118	24.456 23.347	1.00 16.44	A
	ATOM	1514	CA	SER				47.175	25.970 26.228	22.382	1.00 18.49	A
	MOTA	1515	CB	SER				48.340	26.220	23.031	1.00 22.10	A
	MOTA	1516	OG	SER				49.402 46.040	25.257	22.612	1.00 22.10	. A
30	ATOM	1517	С	SER				45.099	25.898	22.148	1.00 17.57	A
	ATOM	1518	0	SER ASP				46.119	23.928	22.517	1.00 16.30	A
	ATOM	1519	N	ASP				45.069	23.166	21.836	1.00 16.72	A
	ATOM	1520 1521	CA CB	ASP				45.483	21.704	21.620	1.00 15.92	A
35	ATOM ATOM	1521	CG	ASP		264		46.544	21.539	20.548	1.00 17.93	A
33	ATOM	1523		ASP				46.642	22.412	19.661	1.00 16.78	A
	ATOM	1524		ASP			•	47.265	20.515	20.579	1.00 16.64	A
	ATOM	1525	C	ASP				43.773	23.194	22.646	1.00 17.67	A
	ATOM	1526	0	ASP				42.681	23.197	22.076	1.00 18.27	A
40	ATOM	1527	Ŋ.	LEU				43.898	23.205	23.974	1.00 15.49	А
	ATOM	1528	CA	LEU				42.730	23.232	24.849	1.00 14.75	Α
	ATOM	1529	CB	LEU	Α	265		43.147	23.038	26.313	1.00 11.38	A
	ATOM	1530	CG			265		43.711	21.641	26.621	1.00 14.04	. A
	ATOM	1531	CD1	LEU	Α	265		44.249	21.579	28.052	1.00 13.96	A
45	ATOM	1532	CD2	LEU	Α	265		42.619	20.603	26.416	1.00 11.62	A
	ATOM	1533	С			265		41.999	24.557	24.675	1.00 15.13	A
	ATOM	1534	0			265		40.777		24.785	1.00 16.75	A
	ATOM	1535	N	TRP	Α	266		42.746		24.405	1.00 16.08	A
	ATOM	1536	CA	TRP	A	266		42.118		24.184	1.00 16.96	A
50	ATOM	1537	CB	TRP	Α	266		43.176		24.023	1.00 17.28	A
	MOTA	1538	CG			266		42.618	29.326	23.521	1.00 20.54	A
	MOTA	1539		TRP				42.313		24.301	1.00 20.07	A
	ATOM	1540	CE2	TRP	Α	266		41.782		23.417	1.00 20.46	A
	ATOM	1541		TRP				42.435		25.660	1.00 20.68	A
55	ATOM	1542		TRP				42.270		22.231	1.00 19.53	A
	ATOM	1543		TRP				41.769		22.163	1.00 19.61	A
•	ATOM	1544		TRP				41.372		23.850	1.00 20.90	A
	MOTA	1545	CZ3	TRP	A	266		42.026		26.091	1.00 19.45	A A
	ATOM	1546	CH2	TRP	A	266		41.501	33.015	25.185	1.00 20.71	A

	MOTA	1547	C	TRP	A	266	41.284	26.795	22.913	1.00	17.22	A
	ATOM '	1548	0	TRP	Α	266	40.139	27.240	22.863	1.00	18.03	A
	ATOM	1549	N	ALA	A	267	41.863	26.181	21.886	1.00	17.50	Α
	ATOM	1550	CA	ALA	Α	267	41.155	25.990	20.626	1.00		A
5	ATOM	1551	CB	ALA	Α	267	42.050	25.290	19.621	1.00	14.28	A
	MOTA	1552	С	ALA	Α	267	39.901	25.159	20.891	1.00		A
	MOTA	1553	0	ALA	Α	267	38.835	25.436	20.346	1.00	16.46	Ά
	MOTA	1554	N	LEU	Α	268	40.031	24.144	21.739	1.00	16.57	A
	ATOM	1555	CA	LEU	Α	268	38.890	23.299	22.084	1.00	17.03	A
10	ATOM	1556	CB	LEU	Α	268	39.292	22.260	23.139	1.00	15.35	A
	ATOM	1557	CG	LEU	Α	268.	38.158	21.429	23.754	1.00		A
	MOTA	1558		LEU			37.505	20.578	22.678	1.00		A
	ATOM	1559		LEU			38.718	20.537	24.881	1.00	17.49	A
	ATOM	1560	С	LEU			37.766	24.179	22.628	1.00	L5.72	A
15	ATOM	1561	0	LEU			36.603	24.031	22.247	1.00		A
	ATOM	1562	N	GLY			38.119	25.099	23.520	1.00	L4.34	Α
	ATOM	1563	CA	GLY			37.124	25.989	24.092	1.00	13.39	A
	MOTA	1564	С	GLY			36.406	26.808	23.031	1.00	L4.94	A
	ATOM	1565	0	GLY			35.193	27.014	23.114	1.00		A
20	ATOM	1566	N	CYS			37.146	27.279	22.030	1.00	L3.86	A
	ATOM	1567	CA	CYS			36.539	28.061	20.958	1.00	L6.80	A
	ATOM	1568	СВ	CYS			37.611	28.634	20.023	1.00		A
	ATOM	1569	SG	CYS			38.751	29.810	20.780	1.00 2		A
	ATOM	1570	С	CYS			35.598	27.175	20.140	1.00		. A
25	ATOM	1571	Ö	CYS			34.516	27.604	19.741	1.00	18.38	A
	MOTA	1572	N	ILE			36.022	25.939	19.887	1.00	16.99	A
	ATOM	1573	CA	ILE			35.221	25.004	19.104	1.00	16.66	A
	MOTA		· CB	ILE	Α	271	36.038	23.741	18.778	1.00 1	16.53	A
	ATOM	1575	CG2	ILE	Α	271	35.155	22.694	18.102	1.00	16.34	A
30	ATOM	1576	CG1	ILE	A	271	37.222	24.129	17.882	1.00	L5.59	A
	ATOM	1577	CD1	ILE	Α	271	38.239	23.018	17.690	1.00	L4.88	A
	ATOM	1578	С	ILE	Α	271	33.920	24.626	19.809	1.00	16.74	A
	MOTA	1579	0	ILE	Α	271	32.865	24.576	19.179	1.00	17.12	A
	MOTA	1580	N	ILE	Α	272	33.990	24.357	21.111	1.00	16.13	A
35	MOTA	1581	CA	ILE	Α	272	32.785	24.021	21.862	1.00	18.30	A
	MOTA	1582	CB	ILE	Α	272	33.097	23.747	23.346	1.00	17.77	A
	ATOM	1583	CG2	ILE '	Α	272	31.796	23.666	24.152	1.00	17.96	A
	MOTA	1584	CG1	ILE	A	272	33.877	22.437	23.481	1.00		A
	ATOM	1585	CD1	ILE	Α	272	34.446	22.217	24.886	1.00	L8.64	Α
40	ATOM	1586	С	ILE	A	272	31.824	25.207	21.776	1.00		A
	MOTA	1587	0	ILE	Α	272	30.624	25.037	21.554	1.00 2		A
	MOTA	1588	N	TYR	Α	273	32.362	26.409	21.947	1.00		A
	MOTA	1589	CA	TYR	Α	273	31.553	27.615	21.881	1.00 2	20.48	A
	MOTA	1590	CB	TYŔ			32.418	28.847	22.162	1.00	18.98	A
45	MOTA	1591	CG	TYR			31.663	30.161	22.125	1.00 2		A
	ATOM	1592	CD1	TYR	Α	273	31.229	30.709	20.916	1.00 2		A
	MOTA	1593	CE1	TYR	A	273	30.536	31.917	20.880	1.00 2		A
	MOTA	1594	CD2	TYR	A	273	31.383	30.857	23.302	1.00		A
	ATOM	1595	CE2	TYR	A	273	30.691	32.062	23.280	1.00 2		A
50	MOTA	1596	CZ	TYR			30.271	32.587	22.067	1.00 2		A
	ATOM	1597	OH	TYR			29.588	33.776	22.049	1.00 2		A
	MOTA	1598	С	TYR			30.902	27.730	20.507	1.00 2		A
	MOTA	1599	0	TYR			29.719	28.049	20.401	1.00 2		A
	ATOM	1600	N	GLN			31.676	27.454	19.461	1.00 2		A
55	ATOM	1601	CA	GLN			31.176	27.538	18.095	1.00 2		A
	ATOM	1602	CB	GLN			32.323	27.341	17.097	1.00 2		A
	ATOM	1603	CG	GLN			31.934	27.596	15.645	1.00 2		A
	ATOM	1604	CD	GLN			33.131	27.588	14.706	1.00 2		A
	ATOM	1605	OE1	GLN	A	274	34.276	27.446	15.139	1.00 2	22.51	A

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	ATOM	1606	NE2	GLN	A	274		32.870	27.750	13.413	1.00 22.96	A
	ATOM	1607	С	GLN	Α	274		30.076	26.517	17.828	1.00 21.51	Ä
	ATOM	1608	0	GLN	A	274		29.123	26.806	17.108	1.00 20.50	Α
	ATOM	1609	N	LEU	Α	275		30.207	25.324	18.403	1.00 21.44	Α
5	ATOM	1610	CA	LEU	Α	275		29.196	24.282	18.208	1.00 20.95	A
	ATOM	1611	СВ	LEU	Α	275		29.645	22.958	18.846	1.00 19.11	A
	ATOM	1612	CG	LEU				30.775	22.182	18.159	1.00 21.43	A
	ATOM	1613		LEU				31.118	20.936	18.963	1.00 17.64	A
	ATOM	1614		LEU				30.342	21.795	16.754	1.00 20.34	A
10	MOTA	1615	C	LEU				27.860	24.697	18.815	1.00 21.32	A
10	ATOM	1616	Ö	LEU				26.802	24.461	18.229	1.00 19.75	A
	ATOM	1617	N	VAL				27.921	25.322	19.987	1.00 19.10	Ą
	ATOM	1618	CA	VAL				26.724	25.750	20.702	1.00 22.47	Ā
	MOTA	1619	CB	VAL				27.011	25.730	22.217	1.00 20.87	A
15	ATOM	1620		VAL				25.742	26.291	22.957	1.00 20.67	A
13		1621		VAL				27.550	24.558	22.766	1.00 19.43	A
	ATOM			VAL				26.127	27.075	20.211	1.00 13.43	A
	ATOM	1622	С								1.00 23.09	A
	MOTA	1623	0	VAL				24.910	27.199	20.070		
	MOTA	1624	N	ALA				26.983	28.062	19.965	1.00 24.56 1.00 24.72	A
20	ATOM	1625	CA	ALA				26.533	29.374	19.518		A
	MOTA	1626	CB	ALA				27.504	30.444	19.999	1.00 24.36	A
	MOTA	1627	C	ALA				26.378	29.458	18.005	1.00 25.76	A
	MOTA	1628	0	ALA				25.577	30.242	17.502	1.00 26.39	A
	MOTA	1629	N	GLY				27.142	28.651	17.280	1.00 25.13	A
25	MOTA	1630	CA	GLY				27.062	28.673	15.834	1.00 25.58	A
	MOTA	1631	С	GLY				28.163	29.524	15.231	1.00 26.50	A
	MOTA	1632	0	GLY			٠	28.374	29.510	14.015	1.00 28.17	A
	MOTA	1633	N	LEU				28.866	30.262	1,6.086	1.00 24.44	A
	ATOM	1634	CA	LEU				29.962	31.130	15.656	1.00 25.21	A
30	MOTA	1635	CB	LEU				29.468	32.575	15.500	1.00 25.78	A
	MOTA	1636	CG	LEU				28.364	32.899	14.490	1.00 28.17	A
	ATOM	1637		LEU				27.922	34.344	14.684	1.00 26.60	A
	MOTA	1638		LEU				28.862	32.670	13.071	1.00 26.52	. A
	MOTA	1639	С	LEU				31.093	31.116	16.687	1.00 23.47	A
35	MOTA	1640	0	LEU				30.848	30.994	17.882	1.00 24.44	A
	MOTA	1641	N	PRO				32.349	31.239	16.236	1.00 23.35	A
	MOTA	1642	CD	PRO				32.831	31.404	14.855	1.00 22.26	A
	MOTA	1643	CA	PRO				33.464	31.239	17.189	1.00 23.81	A
	ATOM	1644	CB	PRO				34.692	31.293	16.282	1.00 23.24	A
40	MOTA	1645	CG	PRO				34.189	32.020	15.073	1.00 24.89	A
	MOTA	1646	С			280		33.353	32.444	18.137	1.00 22.69	A ·
	MOTA	1647	0	PRO			•	32.750	33.457	17.788	1.00 22.11	A
	MOTA	1648	N			281		33.939	32.344	19.345	1.00 23.06	A
	MOTA	1649	CD	PRO				34.810	31.223	19.734	1.00 21.37	A
45	MOTA	1650	CA	PRO				33.935	33.375	20.395	1.00 23.67	A .
	MOTA	1651	CB	PRO				34.781	32.751	21.509	1.00 24.89	A
	ATOM	1652	CG	PRO				34.749	31.287	21.219	1.00 25.24	A
	ATOM	1653	С			281		34.481	34.752	20.017	1.00 23.75	A
	MOTA	1654	0	PRO				33.869	35.781	20.317	1.00 21.02	A
50	MOTA	1655	N	PHE				35.644	34.763	19.379	1.00 22.17	A
	ATOM	1656	CA	PHE				36.293	36.007	18.998	1.00 23.16	, A
	MOTA	1657	CB	PHE				37.765	35.943	19.406	1.00 21.01	A
	ATOM	1658	CG	PHE				37.975	35.482	20.822	1.00 22.66	A ·
	ATOM	1659		PHE				37.806	36.361	21.888	1.00 20.06	A
55	MOTA	1660		PHE				38.291	34.151	21.093	1.00 20.72	A
	MOTA	1661		PHE				37.947	35.921	23.206	1.00 22.66	A
	MOTA .	1662	CE2	PHE				38.433	33.702	22.405	1.00 20.97	A
	ATOM	1663	CZ	PHE				38.261	34.590	23.466	1.00 19.58	A
	MOTA	1664	C	PHE	A	282		36.169	36.263	17.503	1.00 24.39	A

	ATOM	1665	0	PHE	A 282	36.802	35.585	16.694	1.00 25.80	A
	ATOM	1666	N		A 283		37.248	17.142	1.00 23.80	
	ATOM	1667	CA		A 283		37.594	15.741		A
	ATOM	1668	CB		A 283		37.209		1.00 26.33	A
5	ATOM	1669	CG		A 283		35.808	15.316	1.00 28.91	A
,								15.724	1.00 30.27	Α
	ATOM	1670	CD		A 283		35.493	15.188	1.00 33.36	A
	ATOM	1671	NE		A 283		36.392	15.733	1.00 32.76	A
	ATOM	1672	CZ		A 283		36.287	16.952	1.00 34.79	A
10	ATOM			ARG			35.317	17.768	1.00 35.77	A
10	ATOM	1674		2 ARG			37.156	17.359	1.00 36.12	A
	ATOM	1675	С		A 283		39.096	15.544	1.00 26.47	A
	ATOM	1676	0		A 283		39.888	16.438	1.00 26.28	A
• •	ATOM	1677	N		A 284		39.486	14.373	1.00 26.70	· A
	MOTA	1678	CA		A 284		40.899	14.079	1.00 27.84	A
15	MOTA	1679	CB	ALA	A 284	37.188	41.442	14.914	1.00 26.24	A
	ATOM	1680	С	ALA	A 284	36.327	41.077	12.602	1.00 28.35	A
	MOTA	1681	0	ALA	A 284	36.560	40.101	11.891	1.00 29.91	Α
	MOTA	1682	N	GLY	A 285	36.332	42.329	12.153	1.00 29.29	Α
	ATOM	1683	CA	GLY	A 285	36.577	42.631	10.753	1.00 29.52	A
20	MOTA	1684	С	GLY .	A 285	37.893	42.156	10.168	1.00 30.12	A
•	ATOM	1685	0	GLY .	A 285		41.862	8.976	1.00 30.60	A
	ATOM	1686	N		A 286		42.097	10.983	1.00 28.49	A
	ATOM	1687	CA		A 286		41.644	10.489	1.00 26.71	A
	ATOM	1688	CB		A 286		42.825	9.945	1.00 26.71	A
25	ATOM	1689	CG		A 286		43:900	10.990	1.00 27.83	A
	ATOM	1690		ASN			43.631	12.049	1:00 27.84	A
	ATOM	1691		ASN			45.131	10.685	1.00 27.04	A
	ATOM	1692	C		A 286		40.924	11.584	1.00 25.93	
	ATOM	1693	Õ		A 286		40.851	12.723	1.00 25.66	A
30	ATOM	1694	N		A 287		40.831			A
50	ATOM	1695						11.239	1.00 24.81	A
•	ATOM	1696	CA CB		A 287 A 287		39.662	12.206	1.00 27.59	A
		1697					38.985	11.510	1.00 30.17	A
	ATOM		CG		A 287		37.632	10.931	1.00 38.21	A
35	ATOM	1698	CD		A 287		36.998	10.140	1.00 41.86	A
33	ATOM	1699		GLÜ Z			37.036	10.608	1.00 43.08	A
	ATOM	1700	OE2				36.449	9.052	1.00 45.22	A
	ATOM	1701	С		A 287		40.485	13.383	1.00 25.05	A
	ATOM	1702	0		A 287		40.030	14.521	1.00 26.41	A
40	ATOM	1703	N		A 288		41.685	13.122	1.00 23.04	A
40	ATOM	1704	CA		A 288	44.460	42.528	14.205	1.00 22.34	A
	ATOM	1705	CB		1 288	44.867	43.913	13.691	1.00 21.07	A
	ATOM	1706	CG		288	45.275	44.858	14.805	1.00 21.07	A
	ATOM	1707	CD1	TYR A		46.533	44.762	15.405	1.00 21.23	A
	MOTA	1708	CE1	TYR A	1 288	46.891	45.588	16.475	1.00 20.43	A
45	MOTA	1709		TYR A		44.380	45.809	15.302	1.00 22.32	A
	ATOM	1710		TYR A		44.725	46.637	16.373	1.00 23.28	A
	MOTA	1711	CZ	TYR A	288	45.981	46.518	16.953	1.00 22.96	Α
	MOTA	1712	OH	TYR A	288	46.316	47.313	18.024	1.00 23.18	A
	ATOM	1713	C	TYR A	288	43.402	42.698	15.288	1.00 21.38	A
50	ATOM	1714	0	TYR A	288	43.710	42.616	16.473	1.00 22.09	A
	MOTA	1715	N	LEU F	289	42.159	42.939	14.874	1.00 21.88	A
	ATOM	1716	CA	LEU A	289	41.055	43.130	15.811	1.00 21.98	A
	ATOM	1717	CB	LEU F	289	39.821	43.673	15.078	1.00 22.90	A
	ATOM	1718	CG	LEU A	289	39.896	45.130	14.601	1.00 26.52	A
55	ATOM	1719		LEU F		38.706	45.436	13.696	1.00 26.55	A
	ATOM	1720		LEU F		39.914	46.071	15.807	1.00 23.13	A
	ATOM	1721	С	LEU A		40.686	41.849	16.560	1.00 21.24	A
	ATOM	1722	0	LEU P		40.256	41.897	17.715	1.00 20.72	A
	ATOM	1723	N	ILE P		40.843	40.708	15.900	1.00 19.62	A
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	MOTA	1724	CA	ILE A 29	0	40.538	39.433	16.533	1.00 18.54	A
	ATOM	1725	CB	ILE A 29		40.560	38.281	15.509	1.00 18.52	A
	ATOM	1726	CG2			40.503	36.934	16.234	1.00 17.63	A
	MOTA	1727	CG:		0	39.378	38.429	14.545	1.00 18.88	A
5	ATOM	1728	CD:			39.421	37.483	13.357	1.00 19.81	A
	MOTA	1729	. C	ILE A 29)	41.578	39.167	17.618	1.00 19.09	· A
	ATOM	. 1730	0	ILE A 29)	41.236	38.788	18.737	1.00 18.20	A
	MOTA	1731	N	PHE A 29	l	42.849	39.376	17.286	1.00 18.76	A
	ATOM	1732	CA	PHE A 29	L	43.925	39,156.	18.247	1.00 20.75	A
10	ATOM	1733	CB	PHE A 29		45.286	39.434	17.606	1.00 20.71	A
	ATOM	1734	CG	PHE A 29		45.644	38.480	16.503	1.00 22.92	A
	MOTA	1735	CD1	PHE A 29		45.065	37.214	16.443	1.00 22.98	A
	ATOM	1736		PHE A 29		46.588	38.830	15.543	1.00 22.91	A
	ATOM	1737		PHE A 29		45.423	36.310	15.440	1.00 24.51	A
15	ATOM	1738		PHE A 29		46.954	37.931	14.535	1.00-25.54	
	ATOM	1739	CZ	PHE A 29		46.370	36.670	14.485	1.00 23.29	A
	ATOM	1740	C	PHE A 29		43.739	40.061	19.451	1.00 21.72	A
	ATOM	1741	Ó	PHE A 29		43.992	39.671	20.593	1.00 22.32	A
	ATOM	1742	N	GLN A 292		43.284	41.275	19.178	1.00 23.27	A:
20	ATOM	1743	CA	GLN A 292		43.055	42.264	20.216	1.00 24.01	A
	ATOM	1744	СВ	GLN A 292		42.574	43.559	19.562	1.00 25.77	A
	ATOM	1745	CG	GLN A 292		42.577	44.773	20.447	1.00 28.45	A
	ATOM	1746	CD	GLN A 292		42.469	46.057	19.638	1.00 29.83	A
	ATOM	1747		GLN A 292		41.520	46.244	18.872	1.00 27.16	A
25	ATOM	1748		GLN A 292		43.449	46.944	19.799	1.00 27.61	A
	ATOM	1749	С	GLN A 292		42.018	41.733	21.204	1.00 22.97	A
	ATOM	1750	Ō	GLN A 292		42.200	41.832	22.415	1.00 21.64	A
	ATOM	1751	N	LYS A 293		40.937	41.154	20.687	1.00 21.82	A
	ATOM	1752	CA	LYS A 293		39.895	40.612	21.558	1.00 22.18	A
30	ATOM	1753	CB	LYS A 293		38.664	40.223	20.740	1.00 22.69	A
	ATOM	1754	CG	LYS A 293		37.919	41.407	20.153	1.00 25.78	A
	ATOM	1755	CD	LYS A 293		36.651	40.961	19.429	1.00 27.88	A
	ATOM	1756	CE	LYS A 293	1	35.857	42.161	18.926	1.00 30.85	A
	ATOM	1757	NZ	LYS A 293	;	34.612	41.750	18.214	1.00 32.98	A
35	ATOM	1758	С	LYS A 293		40.398	39.398	22.343	1.00 21.20	. A
	MOTA	1759	0	LYS A 293	ı	40.041	39.204	23.509	1.00 22.01	А
	ATOM	1760	N	ILE A 294		41.226	38.583	21.702	1.00 19.91	Α
	ATOM	1761	CA	ILE A 294		41.774	37.394	22.347	1.00 20.28	A
	ATOM	1762	CB	ILE A 294		42.631	36.575	21.349	1.00 18.98	Α
40	MOTA	1763	CG2	ILE A 294		43.481	35.550	22.098	1.00 17.70	Α
	ATOM	1764	CG1	ILE A 294		41.716	35.897	20.318	1.00 17.93	A
	ATOM	1765	CD1	ILE A 294		42.467	35.237	19.178	1.00 16.21	Α
	MOTA	1766	С	ILE A 294		42.618	37.727	23.587	1.00 21.94	· A
	MOTA	1767	0	ILE A 294		42.366	37.199	24.673	1.00 20.86	A
45	MOTA	1768	N	ILE A 295		43.610	38.600	23.439	1.00 21.88	A
	ATOM	1769	CA	ILE A 295		44.461	38.934	24.582	1.00 24.25	. A
	ATOM	1770	CB	ILE A 295		45.668	39.805	24.175	1.00 23.93	A
	ATOM	1771	CG2	ILE A 295	•	46.514	39.066	23.140	1.00 24.61	Α
	MOTA	1772	CG1	ILE A 295		45.189	41.151	23.637	1.00 24.58	A
50	MOTA	1773	CD1	ILE A 295		46.317	42.149	23.433	1.00 26.69	A
	MOTA	1774	С	ILE A 295		43.720	39.636	25.717	1.00 24.80	A
	ATOM	1775	0	ILE A 295		44.214	39.687	26.842	1.00 24.76	A
	MOTA	1776	N	LYS A 296		42.539	40.173	25.425	1.00 25.33	A
	MOTA	1777	CA	LYS A 296		41.743	40.853	26.444	1.00 26.80	A
55	MOTA	1778	СВ	LYS A 296		41.178	42.170	25.894	1.00 27.39	A
	ATOM	1779	CG	LYS A 296		42.240	43.141	25.413	1.00 31.79	A
	ATOM	1780	CD	LYS A 296		41.634	44.410	24.826	1.00 35.56	A
	MOTA	1781	CE	LYS A 296		41.009	45.283	25.900	1.00 39.29	A
	ATOM	1782	NZ	LYS A 296		40.564	46.603	25.357	1.00 41.72	A

	ATOM	1783	С	LYS	A	296		40.593	3	39.958	26.893	1.00	25.50	A
•	ATOM	1784	0	LYS	Α	296		39.770)	40.361	27.713	1.00	24.02	A
	ATOM	1785	N	LEU	Α	297		40.550)	38.742	26.349	1.00	25.67	A
	ATOM	1786	CA	LEU	Α	297		39.500)	37.777	26.666	1.00	25.16	A
5	MOTA	1787	CB	LEU	A	297		39.632	2	37.285	28.111	1.00	24.80	A
	MOTA	1788	CG	LEU	Α	297		38.766	5	36.068	28.460	1.00	26.43	A
	ATOM ·	1789	CD1	LEU	A	297	• •	39.238	3	34.852	27.646		26.70	Α
	ATOM	1790	CD2	LEU	Α	297		38.856	5	35.777	29.951	1.00	24.84	A
	MOTA	1791	С	LEU	A	297		38.151	L	38.459	26.467	1.00	25.11	A
10	MOTA	1792	0	LEU	Α	297		37.261	L	38.378	27.309		25.28	A
	ATOM	1793	N	GLU	A	298		38.007	7	39.127	25.331	1.00	24.98	A
	ATOM	1794	CA	GLU	A	298		36.786	5	39.847	25.023		25.31	. A
	ATOM	1795	CB	GLU	A	298		37.143	3	41.139	24.291		27.13	A
	ATOM	1796	CG	GLU	A	298		35.991	L	42.092	24.108		31.28	A
15	MOTA	1797	CD	GLU	A	298		36.419		43.362	23.410		34.40	A
	MOTA	1798	OE1	GLU	Α	298		37.348		44.027	23.918		35.90	A
	ATOM	1799	OE2	GLU	A	298		35.832	2	43.693	22.359		36.16	A
	MOTA	1800	С	GLU	A	298		35.766	5	39.057	24.207		23.79	A
	MOTA	1801	0	GLU	A	298		35.832	2	39.017	22.979		24.35	A
20	MOTA	1802	N	TYR	A	299		34.825	5	38.427	24.902		23.45	A
	ATOM	1803	CA	TYR	A	299		33.760		37.663	24.265		23.98	A
	MOTA	1804	CB	TYR				34.264		36.304	23.755		20.13	A
	ATOM	1805	CG	TYR				34.348		35.233	24.828		21.17	A
	ATOM	1806	CD1					35.336		35.279	25.810		19.32	A
25	ATOM	1807	CEI			299		35.389		34.332	26.826		19.30	A
	ATOM	1808	CD2					33.410		34.201	24.888		18.96	A
	MOTA	1809	CE2	TYR	A	299		33.456		33.243	25.907		19.41	A
	ATOM	1810	CZ	TYR				34.449		33.321	26.870		18.79	Α.
	MOTA	1811	OH	TYR				34.511		32.401	27.881		18.77	A
30	MOTA	1812	С	TYR				32.699		37.437	25.331		25.20	A
	MOTA	1813	0	TYR				32.942		37.681	26.506		26.46	A
•	MOTA	1814	N	ASP				31.522		36.981	24.927		26.94	A A
	. ATOM	1815	CA	ASP				30.467		36.710	25.891		30.60 35.86	A
	MOTA	1816	CB	ASP				29.665		37.981	26.179		42.04	A
35	MOTA	1817	CG	ASP				29.228		38.687	24.923	-	45.98	A
	ATOM	1818		ASP				28.450		38.088	24.149 24.707		45.69	A
	ATOM	1819		ASP				29.666		39.840 35.608	25.363		29.26	A
	ATOM	1820	С	ASP				29.564 29.590		35.299	24.172		28.64	A
4.0	ATOM	1821	0	ASP				28.778		35.011	26.253		28.96	A
40	MOTA	1822	N			301		27.884		33.924	25.871		30.48	A
	ATOM	1823	CA	PHE				27.818		32.854	26.968		29.17	A
	ATOM	1824	CB			301 301		29.147		32.279	27.356		29.29	A
	ATOM	1825	CG					29.978		32.949	28.245		27.31	A
45	ATOM	1826		PHE				29.560		31.050	26.845		27.89	A
45	ATOM	1827		PHE				31,205		32.403	28.625		28.83	A
	ATOM	1828		PHE PHE				30.78		30.498	27.217		28.05	A
	MOTA	1829 1830	CEZ			301		31.605		31.175	28,110		28.27	Α
	ATOM	1831	C			301		26.459		34.384	25.619		32.20	A
50	ATOM ATOM	1832	0			301		25.946		35.261	26.317		32.36	A
50	ATOM	1833	N			302		25.798		33.804	24.607		33.29	A
		1834	CD			302		26.313		32.943	23.529		34.04	Α
	ATOM ATOM	1835	CA			302		24.419		34.199	24.341		35.24	A
	ATOM	1836	CB			302		24.144		33.608	22.959		34.01	A
55	ATOM	1837	CG			302		25.043		32.413	22.921		35.48	Α
J J	ATOM	1838	C			302		23.56		33.561	25.444		37.39	A
	ATOM	1839	Ö			302		23.93		32.518	25.986		38.49	A
	ATOM	1840	N			303		22.44		34.188	25.783		39.36	A
	ATOM	1841	CA			303		21.572		33.692	26.843	1.00	40.65	A
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	ATOM	1842	СВ	ALA A	303	:	20.280	34.506	26.862		41.66	A
•	ATOM	1843	С	ALA A		:	21.238	32.197	26.814		41.25	A
	ATOM	1844	0	ALA A			21.253	31.537	27.854		43.16	A
	ATOM	1845	N	ALA A	304		20.945	31.665	25.631		41.04	A
5	ATOM	1846	CA	ALA A	304	:	20.569	30.258	25.480	1.00	40.66	A
_	ATOM	1847	CB	ALA A	304		20.121	30.004	24.040	1.00	41.36	Α
	ATOM	1848	С	ALA A			21.628	29.223	25.876		39.61	A
	ATOM	1849	0	ALA A	304		21.298	28.156	26.395	1.00	40.61	A
	ATOM	1850	N	PHE A	305		22.891	29.543	25.617		36.21	A
10	ATOM	1851	CA	PHE A	305		24.022	28.662	25.909		32.08	A
	ATOM	1852	CB	PHE A	305		25.259	29.519	26.187		29.46	A
	ATOM	1853	CG	PHE A	305		26.536	28.917	25.690		28.15	A
	MOTA	1854		PHE A			27.146	27.875	26.377		26.20	A
	MOTA	1855		PHE A			27.127	29.386	24.521		27.05	A
15	ATOM	1856		PHE A			28.330	27.308	25.908		26.92	·A
	ATOM	1857	CE2	PHE A	305		28.312	28.826	24.042		26.62	A
	ATOM	1858	CZ	PHE A	305		28.914	27.786	24.737		26.61	A
	ATOM	1859	С	PHE A	305		23.811	27.664	27.057		30.09	
	ATOM	1860	0	PHE A			23.518	28.051	28.187		31.51	A
20	MOTA	1861	N	PHE A			23.964	26.378	26.758		27.01	A
	MOTA	1862	CA	PHE A			23.801	25.334	27.769		26.30	A A
	MOTA	1863	CB	PHE A			24.157	23.970	27.170		25.03 27.24	A
	ATOM	1864	CG	PHE A			23.548	23.725	25.815		28.40	A
	MOTA	1865		PHE A			22.170	23.831	25.622		27.84	A
25	ATOM	1866		PHE A			24.350	23.386	24.728 24.365		28.05	A
	ATOM	1867		PHE A			21.601	23.603	23.465		28.31	. A
	ATOM	1868		PHE A			23.792	23.155 23.263	23.403		28.00	A
	MOTA	1869	CZ	PHE A			22.415	25.652	28.961		26.23	A
	ATOM	1870	С	PHE A			24.711 25.927	25.775	28.811		25.59	A
30	MOTA	1871	0	PHE A			24.125	25.796	30.163		26.67	A
	MOTA	1872	N	PRO A			22.685	25.625	30.430		27.95	A
	MOTA	1873	CD	PRO A			24.842	26.110	31.405		26.59	A
	ATOM	1874	CA	PRO A			23.795	25.832	32.481		26.14	A
2.5	ATOM	1875	CB CG	PRO A			22.531	26.250	31.803		27.86	A
35	ATOM	1876 1877	Ċ	PRO A			26.145	25.355	31.659		25.58	A
	ATOM	1878	0	PRO A			27.189	25.964	31.900	1.00	22.65	A
	MOTA MOTA	1879	N	LYS A			26.085	24.031	31.620		24.46	A
	ATOM	1880	ĊA	LYS A			27.274	23.232	31.867	1.00	23.91	A
40	ATOM	1881	CB	LYS A			26.887	21.760	32.024	1.00	23.25	A
70	ATOM	1882	CG	LYS A			26.062	21.532	33.285	1.00	28.49	A
	ATOM	1883	CD	LYS A			25.618	20.093	33.466		30.17	A
	ATOM	1884	CE	LYS A	308		24.760	19.973	34.722		33.12	Α
	ATOM	1885	NZ	LYS A	308		24.122	18.636	34.860		34.13	A
45	ATOM	1886	С	LYS A			28.314	23.426	30.769		22.84	A
	ATOM	1887	0	LYS A			29.514	23.411	31.042		22.46	A
	ATOM	1888	N	ALA A			27.861	23.621	29.534		21.59	A
	ATOM	1889	CA	ALA A			28.792	23.848	28.432		20.02	A
	MOTA	1890	CB	ALA A	309		28.056	23.856	27.106		18.80	A
50	MOTA	1891	С	ALA A		•	29.481	25.191	28.662		21.41	A
	ATOM	1892	0	ALA A			30.680	25.335	28.427		21.39	A
	MOTA	1893	N	ARG A			28.717	26.179	29.121		21.39	A
	ATOM	1894	CA	ARG F			29.290	27.494	29.388		22.02	A A
	ATOM	1895	CB	ARG F			28.213	28.479	29.854		22.39	
55	MOTA	1896	CG	ARG P			28.806	29.756	30.436		25.30 28.33	A A
	ATOM	1897	CD	ARG F			27.780	30.852	30.664		30.18	A
	ATOM	1898	NE	ARG A			28.420	32.039	31.230		30.18	A
	ATOM	1899	CZ	ARG A			27.901	33.263	31.203		31.19	A
	ATOM	1900	NH:	l ARG A	¥ 310		26.719	33.477	30.634	1.00	, ,,,,,,	

	ATOM	1901	NH	2 ARG	A 310	28.567	34.277	31.742	1.00 30.49	A
	ATOM	1902	Ċ.		A '310	30.376		30.458	1.00 21.65	A
	ATOM	1903	0	ARG	A 310	31.464	27.949	30.311	1.00 20.36	A
	MOTA	1904	N	ASP	A 311	30.074	26.677	31.541	1.00 19.57	A
5	ATOM	1905	CA	ASP	A 311	31.043	26.512	32.615	1.00 20.18	A
	ATOM	1906	CB		A 311	30.460	25.649	33.739	1.00 20.39	A
	MOTA	1907	CG		A 311	31.439	25.446	34.881	1.00 23.35	A
	ATOM	1908	OD:		A 311	32.158	24.428	34.885	1.00 24.91	A
	ATOM	1909	OD2	2 ASP	A 311	31.500	26.312	35.776	1.00 26.96	A
10	ATOM	1910	C,		A 311	32.322	25.877	32.073	1.00 19.73	A
	ATOM	1911	´0		A 311	33.422	26.289	32.439	1.00 19.30	A
	ATOM.	1912	N	LEU	A 312	32.179	24.891	31.188	1.00 16.32	A
	ATOM	1913	CA		A 312	33.349	24.226	30.611	1.00 16.66	A
	ATOM	1914	СВ		A 312	32.927	23.035	29.744	1.00 16.12	A
15	ATOM	1915	CG		A 312	34.050	22.320	28.974	1.00 14.73	A
	ATOM	1916	CD1		A 312	35.192	21.935	29.912	1.00 14.75	A
	ATOM	1917			A 312	33.477	21.084	28.289	1.00 14.22	A
	ATOM	1918	Ċ		A 312	34.181	25.189	29.774	1.00 14.22	A
	ATOM	1919	Ō		A 312	35.402	25.241	29.910	1.00 16.01	A
20	ATOM	1920	N		A 313	33.515	25.949	28.908	1.00 16.20	Ā
	ATOM	1921	CA		A 313	34.207	26.907	28.058	1.00 15.20	A
	ATOM	1922	CB		A 313	33.216	27.648	27.130	1.00 15.37	A
	ATOM	1923			A 313	33.915	28.796	26.426	1.00 16.42	A
	ATOM	1924			A 313	32.644	26.672	26.103	1.00 17.88	A
25	ATOM	1925	C		A 313	34.960	27.923	28.911	1.00 17.39	A
	ATOM	1926	ō		A 313	36.093	28.294	28.591	1.00 17.33	A
	ATOM	1927	N		A 314	34.342	28.364	30.004	1.00 13.00	A
	ATOM	1928	CA		A 314	34.986	29.331	30.885	1.00 17.01	A
•	ATOM	1929	CB		A 314	34.009	29.816	31.959	1.00 20.43	A
30	ATOM	1930	CG		A 314	32.800	30.550	31.396	1.00 22.14	A
	ATOM	1931	CD		A 314	31.852	31.025	32.478	1.00 20.32	A
	ATOM	1932			A 314	31.580	30.246	33.417	1.00 33.48	A
	ATOM	1933		GLU		31.370	32.173	32.387	1.00 33.40	A
	ATOM	1934	C		A 314	36.217	28.721	31.539	1.00 19.15	A
35	ATOM	1935	ō		A 314	37.134	29.433	31.934	1.00 13.13	A
	ATOM	1936	N		A 315	36.245	27.400	31.651	1.00 19.51	A
	ATOM	1937	CA		A 315	37.394	26.749	32.258	1.00 19.31	A
	ATOM	1938	СВ		A 315	36.946	25.514	33.043	1.00 13.17	A
	ATOM	1939	CG		A 315	36.280	25.885	34.368	1.00 10.64	A .
40	ATOM	1940	CD		A 315	35.653	24.696	35.073	1.00 19.02	A
	ATOM	1941	CE	LYS	315	35.070	25.095	36.427	0.50 21.00	AC1
	ATOM	1942	NZ	LYS	315	36.119	25.552	37.381	0.50 19.53	AC1
	ATOM	1943	С		A 315	38.452	26.393	31.218	1.00 18.96	A
	ATOM	1944	Ö		A 315	39.511	25.873	31.561	1.00 10.30	A
45	ATOM	1945	N		A 316	38.164	26.691	29.950	1.00 17.08	A
	ATOM	1946	CA		A 316	39.102	26.429	28.854	1.00 17.00	A ·
	ATOM	1947	СВ		A 316	38.414	25.636	27.738	1.00 13.41	A
	ATOM	1948	CG		A 316	38.028	24.201	28.115	1.00 13.01	A
	ATOM	1949		LEU Z		37.139	23.597	27.031	1.00 14.33	A
50	ATOM	1950		LEU A		39.302	23.373	28.309	1.00 12.38	A
	MOTA	1951	C	LEU A		39.652	27.743	28.290	1.00 17.12	
	ATOM	1952	ō	LEU A		40.851	27.860	28.023	1.00 17.12	A A
	ATOM	1953	N	LEU A		38.780	28.729	28.105	1.00 16.33	A A
	ATOM	1954	CA	LEU A		39.228	30.022	27.596	1.00 18.27	
55	ATOM	1955	CB	LEU A		38.083	30.752	26.887	1.00 17.52	A A
-	ATOM	1956	CG		317	37.448	29.973	25.727	1.00 18.37	A A
	ATOM	1957		LEU A		36.415	30.851	25.727	1.00 16.81	
	ATOM	1958		LEU F		38.528	29.526	24.741	1.00 16.47	A
	ATOM	1959	C	LEU F		39.745	30.841	28.774	1.00 17.87	A
			•	r	,	22.143	JU.041	20.//4	1.00 10.27	A

	ATOM	1960	0	LEU	A	317	39.078	31.753	29.273	1.00	18.58	A
	MOTA	1961	N	VAL	Α	318	40.937	30.475	29.229	1.00	18.02	ΑĊ
	MOTA	1962	CA			318	41.593	31.141	30.342	1.00	18.85	Α
	ATOM	1963	CB	VAL			41.846	30.153	31.500		19.91	A
5	MOTA	1964		VAL			42.590	30.848	32.634		20.01	Α
	ATOM	1965	CG2	VAL			40.520	29.584	31.990	1.00	19.44	Α
	MOTA	1966	С	VAL			42.923	31.657	29.811		19.67	A
	ATOM	1967	0	VAL			43.690	30.902	29.208		18.26	Α
	MOTA	1968	N	LEU	Α	319	43.197	32.939	30.028	1.00	20.07	Α
10	MOTA	1969	CA	LEU	Α	319	44.436	33.533	29.538		20.98	A
	MOTA	1970	CB	LEU			44.521	35.002	29.968		21.64	Α
	MOTA	1971	CG	LEU			43.418	35.908	29.408		24.38	A
	MOTA	1972		LEU			43.606	37.332	29.935	1.00	23.28	A
	ATOM	1973	CD2	LEU			43.453	35.887	27.875		24.33	Α
15	ATOM	1974	C	LEO	A	319	45.680	32.774	29.994		20.38	Α
	ATOM	1975	0	ΓEΩ			46.568	32.496	29.192		21.34	A
	ATOM	1976	N	ASP			45.742	32.440	31.280		20.22	Α
	MOTA	1977	CA	ASP			46.879	31.707	31.833		20.90	A
	ATOM	1978	CB	ASP			46.842	31.760	33.365		20.76	A
20	MOTA	1979	CG	ASP			48.049	31.102	34.004		21.51	A
	ATOM	1980		ASP			48.669	30.226	33.367		23.46	A
	ATOM	1981		ASP			48.371	31.450	35.159		23.89	A
	ATOM	1982	С	ASP			46.814	30.247	31.367		20.06	Α.
	ATOM	1983	0	ASP			45.988	29.476	31.840		20.54	A
25	MOTA	1984	N	ALA			47.700	29.876	30.451		20.68	A
	MOTA	1985	CA	ALA			47.733	28.522	29.903		22.04	A
	ATOM	1986	CB	ALA			48.860	28.411	28.881		20.75	A
	ATOM	1987	C	ALA			47.858	27.400	30.940		21.62	A
	ATOM	1988	0	ALA			47.482	26.259	30.665		21.99	A
30	MOTA	1989	N	THR			48.372	27.715	32.127		20.89	A
	MOTA	1990	CA	THR			48.531	26.698	33.167		20.82	A
	MOTA	1991	CB	THR			49.670	27.051	34.146		19.47	A
	MOTA	1992		THR			49.341	28.253	34.848		20.19	A
	MOTA	1993		THR			50.981	27.249	33.394		21.59	A
35	MOTA	1994	C	THR			47.264	26.498	33.983		19.55	A
	ATOM	1995	0	THR			47.235	25.673	34.894		21.13	A
	ATOM	1996	N	LYS			46.216	27.248	33.661		19.33	A
	ATOM	1997	CA	LYS			44.962	27.122	34.392		21.20 23.75	A A
40	ATOM	1998	CB	LYS			44.580	28.460	35.030		28.45	A
40	ATOM	1999	CG	LYS LYS			45.562	28.933	36.084 36.799		33.76	A
	ATOM	2000	CD	LYS			45.055	30.177 30.678	37.802		36.15	A
	ATOM	2001	CE				46.087 46.532	29.569	38.693		37.34	A
	ATOM	2002	NZ C	LYS LYS			43.806	26.614	33.539		20.68	A
15	ATOM	2003	-	LYS			42.649	26.757	33.915		.20.42	A
45	ATOM	2004	0				44.114	26.019	32.392		19.97	A
	ATOM	2005	N	ARG			43.060	25.494	31.531		17.98	A
	ATOM	2006	CA	ARG ARG			43.461	25.609	30.061		15.95	A
	ATOM	2007 2008	CB CG	ARG			43.461	27.050	29.603		17.34	A
50	ATOM			ARG			43.996	27.194	28.172		19.80	A
50	ATOM	2009 2010	CD NE	ARG			44.438	28.565	27.944		16.93	A
	ATOM		CZ	ARG			45.410	28.908	27.108		19.88	A
	ATOM	2011 2012		ARG			46.045	27.978	26.398		14.58	A
	ATOM ATOM	2012		ARG			45.774	30.181	27.015		16.51	A
55	ATOM	2013	C	ARG			42.762	24.046	31.883		18.32	A
<i></i>	ATOM	2014	0	ARG			43.673	23.222	32.006		18.20	A
	ATOM	2015	N	LEU			41.479	23.748	32.055		18.32	A
	ATOM	2017	CA	LEU			41.050	22.403	32.395		17.79	A
		2017	CB	LEU			39.523	22.335	32.425		17.03	A
	ATOM	2010	CD	٥٠٠٠	~	525	37.323	22.333	J2.72J	2.00		

	ATOM	2019	CG	LEU	Α :	325	38.896	21.125	33.116	1.00 15.9	1 A
	ATOM	2020		LEU			39.392	21.048	34.557	1.00 15.9	
	ATOM	2021		LEU			37.375	21.255	33.084	1.00 16.5	
	MOTA	2022	С	LEU	A 3	325	41.599	21.433	31.356	1.00 18.6	
5	ATOM	2023	0	LEU .	A 3	325	41.347	21.586	30.157	1.00 18.2	8 A
	MOTA	2024	N	GLY	A 3	326	42.354	20.439	31.821	1.00 18.1	8 A
	ATOM	2025	CA	GLY			42.931	19.462	30.915	1.00 16.3	
	ATOM	2026	C				44.443	19.558	30.807	1.00 19.1	
				GLY							
	MOTA	2027	0	GLY .			45.093	18.592	30.404	1.00 19.5	
10	MOTA	2028	N	CYS .	A 3	327	45.016	20.708	31.161	1.00 18.1	6 A
	ATOM	2029	CA	CYS .	A 3	327	46.463	20.867	31.075	1.00 19.3	0 · A
	ATOM	2030	CB	CYS .			46.856	22.350	31.058	1.00 20.2	2 A
	ATOM	2031	SG	CYS .			46.782	23.200	32.649	1.00 21.9	
	•										
	ATOM	2032	C	CYS .			47.169	20.157	32.228	1.00 20.2	
15	ATOM	2033	0	CYS .			46.561	19.828	33.246	1.00 17.9	
	ATOM	2034	И.	GLU .	A 3	328	48.463	19.933	32.053	1.00 20.5	1 A
	ATOM	2035	CA	GLU .	A 3	328	49.274	19.244	33.042	1.00 23.3	4 A
	ATOM	2036	СВ	GLU .	A 3	328	50.710	19.139	32.507	1.00 28.6	8 A
	ATOM	2037	CG	GLU .			50.754	18.367	31.175	1.00 38.2	
20				GLU .				18.500	30.414	1.00 43.2	
20	ATOM	2038	CD				52.067				
	ATOM	2039		GLU			52.535	19.643	30.218	1.00 46.2	
	MOTA	2040	OE2	GLU .	А З	328	52.618	17.459	29.991	1.00 44.9	0 A
	ATOM	2041	С	GLU .	A 3	328	49.234	19.876	34.435	1.00 22.1	1 A
	ATOM	2042	0	GLU :			49.147	19.161	35.437	1.00 20.2	7 A
25	ATOM	2043	N	GLU			49.276	21.204	34.506	1.00 18.4	
23				GLU .			49.248	21.875	35.801	1.00 20.1	
	ATOM	2044	CA								
	ATOM	2045	CB	GLU .			49.587	23.363	35.657	1.00 20.3	
	ATOM	2046	CG	GLU .	A 3	329	51.014	23.651	35.190	1.00 24.0	
	ATOM	2047	CD	GLU .	А З	329 .	51.191	23.518	33.688	1.00 25.9	3 A
30	ATOM	2048	OE1	GLU .	A 3	329	50.213	23.154	32.995	1.00 26.6	1 A
	ATOM	2049		GLU			52.311	23.781	33.198	1.00 27.1	9 A
		2050	C	GLU .			47.890	21.718	36.480	1.00 19.3	
	ATOM								37.694	1.00 18.7	
	ATOM	2051	0	GLU .			47.775	21.879			
	ATOM	2052	N	MET .			46.863.	21.415	35.691	1.00 17.2	
35	MOTA	2053	CA	MET .	A 3	330	45.520	21.220	36.229	1.00 16.3	
	ATOM	2054	CB	MET .	A 3	330	44.474	21.833	35.294	1.00 17.6	5 A
	MOTA	2055	CG	MET .	А 3	330	44.460	23.365	35.311	1.00 22.9	5 A
	ATOM	2056	SD	MET .		-	44.186	24.026	36.979	1.00 26.7	8 A
	ATOM	2057	CE	MET .			42.435	23.712	37.186	1.00 24.6	
40				MET .			45.257	19.730	36.422	1.00 14.3	
40	MOTA	2058	С								
	MOTA	2059	0	MET .			44.127	19.304	36.629	1.00 15.3	
	MOTA	2060	N	GLU .	A 3	331	46.327	18.949	36.346	1.00 15.6	
	ATOM	2061	CA	GLU .	А. З	331	46.289	17.501	36.531	1.00 17.0	
	MOTA	2062	CB	GLU :	A 3	331	45.607	17.155	37.862	1.00 17.0	0 A
45	ATOM	2063	CG	GLU .	A 3	331	46.070	18.027	39.038	1.00 17.4	6 A
	ATOM	2064	CD	GLU .			47.591	18.179	39.145	1.00 20.1	
									39.896	1.00 21.3	
	MOTA	2065		GLU .			48.034	19.073			
	ATOM	2066	OE2	GLU .			48.345	17.420	38.500	1.00 18.8	
	ATOM	2067	С	GLU :	ΑЗ	331	45.697	16.658	35.398	1.00 17.8	0 A
50	MOTA	2068	0	GLU .	A 3	331	45.107	15.602	35.636	1.00 20.4	0 A
	MOTA	2069	N	GLY :			45.844	17.133	34.167	1.00 16.2	3 A
	ATOM	2070	CA	GLY .			45.420	16.353	33.015	1.00 14.1	
									32.596	1.00 13.5	
	ATOM	2071	С	GLY .			43.982	16.154			
	MOTA	2072	0	GLY .			43.063	16.864	33.017	1.00 11.9	
55	ATOM	2073	N	TYR .			43.804	15.141	31.750	1.00 14.3	
	ATOM	2074	CA	TYR .	A 3	333	42.510	14.806	31.182	1.00 13.5	6 A
	ATOM	2075	CB	TYR			42.722	13.892	29.968	1.00 15.0	0 A
	ATOM	2076	CG	TYR			43.153	14.683	28.752	1.00 16.4	
				TYR .			42.206	15.172	27.849	1.00 15.2	
	MOTA	2077	CDI	IIN.	- J	,,,,	12.200	10.112	27.047	20.2	_ ••

	ATOM	2078	CE1	TYR	А	333	42.573	16.002	26.794	1.00 13.42	Α
	ATOM	2079	CD2			333	44.490	15.039	28.561	1.00 14.91	
		2080	CE2			333					
	ATOM						44.872	15.877	27.499	1.00 14.87	
_	ATOM	2081	CZ			333	43.902	16.353	26.626	1.00 15.61	
5	ATOM	2082	ОН			333	44.244	17.197	25.599	1.00 17.29	
	ATOM	2083	С	TYR	Α	333	41.470	14.230	32.127	1.00 15.23	A
	ATOM	2084	0	TYR	Α	333	40.278	14.323	31.846	1.00 16.63	A
	ATOM	2085	N	GLY	A	334	41.907	13.650	33.244	1.00 15.50	A
	ATOM	2086	CA	GLY	Α	334	40.957	13.100	34.202	1.00 15.07	A
10	ATOM	2087	С	GLY			39.925	14.146	34.616	1.00 16.40	
	ATOM	2088	ō	GLY			38.724	13.946	34.433	1.00 15.05	
	ATOM	2089	N	PRO			40.366	15.278	35.184	1.00 13.05	
	ATOM	2090	CD	PRO			41.727	15.531	35.689	1.00 15.88	
	ATOM.	2091	CA	PRO			39.444	16.339	35.606	1.00 15.29	
15	ATOM	2092	CB	PRO			40.383	17.397	36.178	1.00 13.19	A
	ATOM	2093	ÇG	PRO	A	335	41.485	16.569	36.758	1.00 13.81	A
	ATOM	2094	С	PRO	Α	335	38.594	16.877	34.448	1.00 15.84	A
	ATOM	2095	0	PRO	Α	335	37.423	17.204	.34.631	1.00 14.84	A
	ATOM	2096	N	LEU	Α	336	39.184	16.971	33.257	1.00 16.12	A
20	ATOM	2097	CA	LEU			38.450	17.465	32.094	1.00 15.52	
20	ATOM	2098	CB '	LEU			39.396	17.653	30.898	1.00 14.39	
			CG	LEU			38.770	17.991	29.538	1.00 15.46	
	ATOM	2099					37.836	19.182	29.662	1.00 13.40	A
	ATOM	2100		LEU							
	MOTA	2101		LEU			39.884	18.285	28.528	1.00 14.11	
25	ATOM	2102	С	LEU			37.321	16.508	31.714	1.00 16.28	A
	ATOM	2103	0	LEU.	Α	336	36.176	16.921	31.540	1.00 15.51	A
	ATOM	2104	N	LYS	Α	337	37.640	15.225	31.592	1.00 17.22	A
	ATOM	2105	CA	LYS	Α	337	36.624	14.243	31.235	1.00 17.39	A
	ATOM	2106	CB	LYS	Α	337	37.293	12.900	30.921	1.00 17.68	A
30	ATOM	2107	CG	LYS			38:170	12.994	29.676	1.00 22.31	Α
50	ATOM	2108	CD	LYS			39.213	11.892	29.592	1.00 24.60	A
	ATOM	2109	CE	LYS			38.620	10.560	29.189	1.00 24.76	
		2110		LYS			39.710	9.560	28.997	1.00 25.05	
	ATOM		NZ				35.577	14.096	32.342	1.00 17.33	
	ATOM	2111	C '	LYS							
35	MOTA	2112	0	LYS			34.456	13.652	32.090	1.00 14.42	
	MOTA	2113	N	ALA			35.928	14.500	33.559	1.00 15.83	
	ATOM	2114	CA	ALA	Α	338	34.989	14.395	34.674	1.00 17.52	
	ATOM	2115	CB	ALA	Α	338	35.749	14.167	35.980	1.00 19.68	A
	ATOM	2116	С	ALA	Α	338	34.095	15.621	34.804	1.00 18.83	
40	ATOM	2117	0	ALA	A	338	33.252	15.687	35.695	1.00 18.94	A
	ATOM	2118	N	HIS			34.262	16.596	33.918	1.00 19.42	A
	ATOM	2119	CA	HIS			33.438	17.796	34.004	1.00 19.28	Α
•	ATOM	2120	CB	HIS			33.865	18.819	32.949	1.00 19.20	Α
	ATOM	2121		HIS			33.163	20.134	33.074	1.00 20.26	
45								21.299	33.649	1.00 18.95	A
45	ATOM	2122		HIS			33.549		32.612	1.00 10.33	A
	MOTA	2123		HIS			31.880	20.340			
	ATOM	2124		HIS			31.506	21.576	32.896	1.00 22.19	
	ATOM	2125	NE2	HIS			32.500	22.179	33.525	1.00 21.98	A
	MOTA	2126	С	HIS	Α	339	31.957	17.448	33.845	1.00 19.13	Α
50	ATOM	2127	0	HIS	Α	339	31.597	16.576	33.061	1.00 19.52	A
	ATOM	2128	N	PRO	Α	340	31.079	18.125	34.606	1.00 19.80	A
	MOTA	2129	CD	PRO	Α	340	31.424	19.119	35.640	1.00 19.08	Α
	ATOM	2130	CA	PRO			29.630	17.900	34.569	1.00 20.52	Α
	ATOM	2131	CB ·	PRO			29.091	19.058	35.396	1.00 20.74	A
55		2131	CG	PRO			30.146	19.207	36.454	1.00 19.20	A
رر	MOTA							17.834	33.176	1.00 13.20	A
	ATOM	2133	C	PRO			29.000			1.00 21.42	A
	MOTA	2134	0	PRO			28.049	17.088	32.955		
	MOTA	2135	N	PHE			29.528	18.606	32.237	1.00 21.33	
	MOTA	2136	CA.	PHE	Α	341	28.985	18.610	30.886	1.00 21.57	A
			•								

	ATOM	2137	CB PHE A	341	29.739	19.624	30.017	1.00 21.64	А
	ATOM	2138	CG PHE A	341 .	29.207	19.740	28.613	1.00 23.18	. A
	ATOM	2139			27.903	20.171	28.382	1.00 23.10	
	ATOM	2140	CD2 PHE A		30.013	19.431	27.522		A
5	ATOM	2141	CE1 PHE A		27.410			1.00 21.95	A
,	ATOM	2142	CE2 PHE A		29.533		27.082	1.00 23.54	A
						19.548	26.220	1.00 21.83	. А
	ATOM	2143	CZ PHE A		28.228	19.980	25.998	1.00 23.23	A
	ATOM	2144	C PHE A		29.055	17.226	30.237	1.00 21.84	A
10	ATOM	2145	O PHE A		28.232	16.896	29.389	1.00 20.37	A
10	ATOM	2146	N PHE A		30.034	16.422	30.640	1.00 20.51	A
	ATOM	2147	CA PHE A		30.221	15.085	30.077	1.00 23.01	Α
	ATOM	2148	CB PHE A	342	31.710	14.809	29.850	1.00 18.00	Α
	ATOM	2149	CG PHE A	342	32.398	15.812	28.971	1.00 17.05	А
	MOTA	2150	CD1 PHE A	342	32.010	15.987	27.652	1.00 17.78	A
15	ATOM	2151	CD2 PHE A	342	33.487	16.534	29.450	1.00 15.72	A
	ATOM	2152	CE1 PHE A	342	32.702	16.867	26.811	1.00 18.08	A
	ATOM	2153	CE2 PHE A		34.184	17.414	28.617	1.00 17.45	A
	ATOM	2154	CZ PHE A		33.790	17.578	27.298	1.00 17.45	A
	ATOM	2155	C PHE A		29.679	13.972	30.976		
20	MOTA	2156	O PHE A		30.002			1.00 24.95	A
20	ATOM	2157				12.798	30.777	1.00 23.95	A
			N GLUA		28.861	14.333	31.958	1.00 27.35	A
	ATOM	2158	CA GLU A		28.325	13.349	32.897	1.00 30.28	A
	ATOM	2159	CB GLU A		27.187	13.964	33.716	1.00 32.20	A
0.5	ATOM	2160	CG GLU A		26.581	12.991	34.714	1.00 39.71	A
25	ATOM	2161	CD GLU A		25.628	13.661	35.688	1.00 44.72	A
	MOTA	2162	OE1 GLU A		24.661	14.314	35.234	1.00 47.55	A
	ATOM	2163	OE2 GLU A		25.847	13.526	36.911	1.00 46.89	A
	ATOM	2164	C GLU A	343	27.852	12.017	32.305	1.00 28.98	Α
	ATOM	2165	O GLU A	343	28.225	10.952	32.800	1.00 31.73	A
30	MOTA	2166	N SER A	344	27.037	12.067	31.258	1.00 26.09	A
	ATOM	2167	CA SER A	344	26.520	10.838	30.656	1.00 28.36	A
	ATOM	2168	CB SER A	344	25.129	11.089	30.067	1.00 28.73	A
	MOTA	2169	OG SER A		25.203	11.942	28.940	1.00 30.91	. A
	ATOM	2170	C SER A		27.407	10.214	29.577	1.00 27.66	A
35	ATOM	2171	O SER A		26.987	9.281	28.900	1.00 28.66	A
	ATOM	2172	N VAL A		28.627	10.715	29.419	1.00 26.75	
	ATOM	2173	CA VAL A		29.534	10.713	28.402		A
	ATOM	2174	CB VAL A		30.565	11.256		1.00 23.44	A
	ATOM	2175	CG1 VAL A				27.950	1.00 23.10	A
40	ATOM	2176	CG2 VAL A		31.589	10.631	26.995	1.00 22.24	A
40					29.854	12.418	27.275.		A
	MOTA	2177	C VAL A		30.326	8.957	28.855	1.00 24.26	A
	ATOM	2178	O VAL A		30.876	8.930	29.960	1.00 22.83	A
	ATOM	2179	N THR A		30.374	7.942	27.997	1.00 21.77	A
	ATOM	2180	CA THR A		31.153	6.740	28.272	1.00 23.70	A
45	ATOM	2181	CB THR A		30.391	5.455	27.857	1.00 26.53	A
	ATOM	2182	OG1 THR A		29.248	5.284	28.706	1.00 29.98	A
	ATOM	2183	CG2 THR A	346 ·	31.289	4.231	27.990	1.00 24.28	A
	ATOM	2184	C THR A	346	32.383	6.945	27.385	1.00 23.43	A
	ATOM	2185	O THR A	346	32.306	6.827	26.160	1.00 24.50	A
50	ATOM	2186	N TRP A		33.508	7.270	28.013	1.00 22.98	A
	ATOM	2187	CA TRP A		34.744	7.569	27.300	1.00 23.81	A
	ATOM	2188	CB TRP A		35.683	8.352	28.219	1.00 23.01	A
	ATOM	2189	CG TRP A		35.128	9.658	28.693	1.00 22.54	A
	ATOM	2190	CD2 TRP A		35.257	10.927			
55	ATOM	2190	CE2 TRP A				28.040	1.00 19.11	A
J.J					34.581	11.881	28.838	1.00 18.39	A
	ATOM	2192	CE3 TRP A 3		35.878	11.351	26.858	1.00 18.16	A
	ATOM	2193	CD1 TRP A 3		34.397	9.883	29.828	1.00 18.35	A
	ATOM	2194	NE1 TRP A 3		34.065	11.218	29.923	1.00 19.51	A
	ATOM	2195	CZ2 TRP A 3	347	34.510	13.234	28.491	1.00 16.88	A

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	ATOM	2196	CZ3	TRP .	A 347	35.808	12.701	26.511	1.00 17.23	A
	ATOM	2197	CH2	TRP .	A 347	35.127	13.624	27.327	1.00 18.16	A
	MOTA	2198	С	TRP :	A 347	35.538	6.429	26.675	1.00 25.79	A
	ATOM	2199	0	TRP .	A 347	36.304	6.654	25.742	1.00 24.67	Α
5	ATOM	2200	N	ALA .	A 348	35.360	5.215	27.183	1.00 27.10	Α
	ATOM	2201	CA	ALA .	A 348	36.116	4.063	26.697	1.00 27.46	Α
	MOTA	2202	CB	ALA	A 348	35.899	2.869	27.636	1.00 27.09	А
	ATOM	2203	С	ALA .	A 348	35.895	3.620	25.256	1.00 27.18	A
	ATOM	2204	0	ALA	A 348	36.830	3.148	24.613	1.00 29.41	A
10	ATOM	2205	N	ASN 2	A 349	34.682	3.769	24.735	1.00 26.55	A
	ATOM	2206	CA	ASN 2	A 349	34.418	3.310	23.375	1.00 27.28	A
	ATOM	2207	CB	ASN 2	A 349	33.700	1.962	23.444	1.00 29.37	A
	ATOM	2208	CG	ASN 2	A 349	32.299	2.088	24.013	1.00 30.92	A
	ATOM	2209	OD1	ASN 3	A 349	32.045	2.942	24.859	1.00 30.17	A
15	ATOM	2210	ND2	ASN A	A 349	31.386	1.237	23.553	1.00 33.52	A
	MOTA	2211	С	ASN A	A 349	33.599	4.265	22.509	1.00 26.47	A
	ATOM	2212	0	ASN 2	A 349	32.669	3.843	21.819	1.00 25.87	A
	ATOM .	2213	N	LEU Z	350	33.947	5.543	22.518	1.00 24.45	A
	ATOM	2214	CA	LEU A	A 350	33.203	6.510	21.721	1.00 23.14	A
20	ATOM	2215	CB	LEU Z	A 350	33.837	7.898	21.848	1.00 23.22	A
	ATOM	2216	CG	LEU A	A 350	33.659	8.605	23.191	1.00 21.05	A
	ATOM	2217	CD1	LEU A	A 350	34.646	9.756	23.293	1.00 19.36	A
	ATOM	2218	CD2	LEU 2	350	32.220	9.094	23.319	1.00 18.78	A
	ATOM	2219	C	LEU Z	¥ 350	33.082	6.152	20.240	1.00 22.60	A
25	ATOM	2220	0	LEU I	350	32.011	6.296	19.650	1.00 21.15	A
	ATOM .	2221	N	HIS 2	351	34.165	5.689	19.627	1.00 23.13	A
	ATOM	2222	CA	HIS 2	351	34.089	5.387	18.204	1.00 27.83	A
	ATOM	2223	CB	HIS 2	351	35.506	5.325	17.596	1.00 29.36	A
	ATOM	2224	CG	HIS 2	351	36.082	3.950	17.493	1.00 32.07	A
30	MOTA	2225	CD2	HIS Z	351	36.611	3.128	18.431	1.00 32.39	A
	ATOM	2226	ND1	HIS 2	A 351	36.197	3.285	16.291	1.00 33.02	A
	ATOM	2227	CE1	HIS 2	A 351	36.775	2.113	16.493	1.00 33.58	A
	MOTA	2228	NE2	HIS 2	351	37.036	1.992	17.782	1.00 31.76	A
	MOTA	2229	С		A 351		4.144	17.874	1.00 28.12	A
35	ATOM	2230	0		351	33.015	3.847	16.707	1.00 29.49	A
	ATOM	2231	N		A 352	32.800	3.442	18.908	1.00 29.28	A
	ATOM	2232	CA	GLN 3	A 352	31.963	2.255	18.726	1.00 29.67	A
	MOTA	2233	CB	GLN	352	32.366	1.145	19.694	0.50 30.56	AC1
	MOTA	2234	CG	GLN	352	33.169	0.041	19.041	0.50 30.88	AC1
40	ATOM	2235	CD	GLN	352	34.493	-0.186	19.729	0.50 31.21	AC1
	MOTA	2236		GLN	352	34.541	-0.450	20.928	0.50 30.76	AC1
	ATOM	2237	NE2		352	35.578	-0.084	18.971	0.50 32.30	AC1
	ATOM	2238	С		352	30.504	2.638	18.963	1.00 30.42	A
	ATOM	2239	0		352	29.595	1.831	18.770	1.00 29.01	A
45	ATOM	2240	N		1 353	30.290	3.875	19.397	1.00 27.64	A
	ATOM	2241	CA		353	28.948	4.365	19.652	1.00 27.42	A
	ATOM	2242	CB		1 353	28.977	5.401	20.775	1.00 25.77	A
	ATOM	2243	CG		4 353	29.408	4.837	22.115	1.00 27.34	A
	ATOM	2244	CD		353	29.638	5.914	23.156	1.00 27.19	A
50	ATOM	2245		GLN Z		28.875	6.872	23.252	1.00 28.29	A
	ATOM	2246		GLN 2		30.687	5.753	23.951	1.00 28.79	A
	ATOM	2247	С		353	28.375	4.989	18.385	1.00 29.00	. A
	ATOM	2248	O.		353	29.118	5.455	17.516	1.00 29.14	· A
	ATOM	2249	N		A 354	27.053	4.984	18.276	1.00 27.31	A n
55	ATOM	2250	CA		354	26.390	5.568	17.119	1.00 27.85	A
	ATOM	2251	CB		354	24.991	4.941	16.904	1.00 30.69	A
	ATOM	2252		THR A		25.132	3.532	16.665	1.00 30.07	A
	MOTA	2253		THR		24.289	5.585	15.709	1.00 29.58	A
	MOTA	2254	С	THR I	A 354	26.244	7.062	17.376	1.00 26.85	A

	ATOM	2255	0	THR	Α	354	25.592	7.475	18.329	1.00 25.77	А
	ATOM	2256	N	PRO	Α	355	26.867	7.898	16.533	1.00 27.22	A
	MOTA	2257	CD			355	27.792	7.588	15.431	1.00 25.89	A
	ATOM	2258	CA	PRO	Α	355	26.763	9.346	16.734	1.00 27.23	A
5	ATOM	2259	СВ	PRO	A	355	27.625	9.915	15.609	1.00 24.91	. A
•	ATOM	2260	CG			355	28.643	8.838	15.385	1.00 25.54	A
	ATOM	2261	С			355	25.322	9.837	16.641	1.00 28.07	A
	ATOM	2262	Ō			355	24.548	9.364	15.810	1.00 27.24	A
	ATOM	2263	N			356	24.941	10.792	17.500	1.00 28.28	A
10	MOTA	2264	CD			356	25.752	11.560	18.462	1.00 28.31	A
	ATOM	2265	CA			356	23.572	11.306	17.448	1.00 28.44	A
	ATOM	2266	CB			356	23.539	12.301	18.604	1.00 28.11	A
	ATOM	2267,	CG			356	24.946	12.832	18.612	1.00 26.86	A
	ATOM	2268	C			356	23.363	11.978	16.097	1.00 29.25	A
15 :		2269	Ö			356	24.304	12.537	15.529	1.00 27.27	A
15 .	ATOM	2270	N			357	22.143	11.910	15.575	1.00 27.27	A
	ATOM	2271	CA	ALA			21.848	12.521	14.287	1.00 30.43	A
	ATOM	2272	CB	ALA			20.507	12.019	13.757	1.00 31.99	A
	ATOM	2273	C	ALA			21.824	14.035	14.448	1.00 31.99	A
20	ATOM	2274	0	ALA			21.194	14.561	15.369	1.00 35.04	A
20	ATOM	2275	Ŋ	LEU			22.516	14.730	13.552	1.00 37.81	A
		2276	CA	LEU			22.578	16.185	13.552	1.00 37.81	A
	ATOM	2277	CB			358	23.679	16.681	12.658	1.00 42.13	A
	ATOM		CG	LEU				16.285	13.109	1.00 39.51	Ā
25	ATOM	2278		LEU			25.086 26.102	16.285	12.062	1.00 39.31	A
25	MOTA	2279							14.445	1.00 39.29	A
	ATOM	2280		LEU			25.395 21.241	16.953	13.242	1.00 45.91	A
	ATOM	2281	C			358		16.837		1.00 45.71	A
	ATOM	2282	0	LEU			20.874 20.530	16.927 17.290	12.069 14.275	1.00 45.71	A. A
20	ATOM	2283	N			359				1.00 53.73	A
30	MOTA	2284	CA			359	19.223	17.939	14.140 13.726	1.00 54.04	A
	ATOM	2285	CB			359	19.353	19.428		1.00 54.04	A
	MOTA	2286		THR			19.995	19.521 20.204	12.448 14.763	1.00 54.32	A
	ATOM	2287		THR			20.158	17.236	13.139	1.00 54.47	A
2.5	ATOM	2288	C			359	18.309		12.930	1.00 54.47	A
35	MOTA	2289	0			359	18.483 17.407	16.016 17.908	12.595	1.00 56.97	A
•	ATOM	2290		THR		359	42.566	19.118	34.302	1.00 30.97	S
	ATOM	2291		TIP		2	41.052	32.378	19.857	1.00 15.82	s
	ATOM	2292			S	3	37.014	33.030	17.747	1.00 15.02	s
40	ATOM	2293			S	5	45.353	24.370	18.152	1.00 16.85	S
40	ATOM	2294	OH2		-	6	31.896	13.930	33.235	1.00 20.42	S
	ATOM	2295		TIP	S	7	50.351	22.781	28.249	1.00 20.42	S
	ATOM	2296 2297			S	8	45.246	-0.589	-0.734	1.00 21.14	s
	ATOM	2298		TIP		11	46.249	-0.348	-8.523	1.00 17.74	S
15	ATOM						45.756	11.148	29.680	1.00 21.94	s
45	ATOM	2299		TIP		14	44.273	13.157	34.592	1.00 21.54	S
	ATOM	2300		TIP TIP		15 17	53.598	3.722	-1.720	1.00 13.01	S
	ATOM	2301					46.049	13.087	31.565	1.00 21.45	· S
	ATOM	2302		TIP		18	53.422	22.401	-3.280	1.00 23.26	S
50	ATOM	2303		TIP		19 20	34.587	7.922	5.383	1.00 23.20	S
50	ATOM	2304		TIP			45.053	27.379	19.376	1.00 22.50	S
	ATOM	2305		TIP.		21	28.899	36.416		1.00 29.00	S
	ATOM.	2306		TIP		23			28.633 -8.219	1.00 31.88	S
	ATOM	2307		TIP		24	35.531	11.645		1.00 23.45	S
<i>e</i> -	ATOM	2308		TIP		25	47.364	28.787	19:612	1.00 23.03	S
55	ATOM	2309		TIP		27	48.859	21.588	12.634	1.00 23.76	S
	ATOM	2310		TIP		29	48.805 48.619	8.920	23.626 10.112	1.00 22.23	S
	ATOM	2311		TIP		31		7.247		1.00 21.32	S
	ATOM	2312		TIP		34	44.824	28.720	15.621	1.00 25.27	S
	ATOM	2313	OHZ	TIP	3	35	26.030	12.634	13.407	1.00 21.01	ລ

	MOTA	2314	OH2 TIP	s 36	50.462	19.810	40.066	1.00 25.45	s
	ATOM	2315	OH2 TIP	s 37	39.631	23.510	-0.239	1.00 30.88	s
	ATOM	2316		S 40		42.655	10.346	1.00 30.84	s
	ATOM	2317	OH2 TIP			3.902	1.503	1.00 27.14	S
5	ATOM	2318		S 45		21.923	39.754	1.00 27.14	
,	ATOM	2319		S 47	47.820	16.413		•	s
		2320	OH2 TIP				7.805	1.00 25.73	. S
	ATOM				50.292	31.412	29.642	1.00 32.79	s
	MOTA	2321		S 49		16.646	34.827	1.00 29.80	S
10	ATOM	2322		S 52	31.714	10.996	31.855	1.00 29.15	S
10	ATOM	2323	OH2 TIP		46.108	23.843	-4.299	1.00 24.21	S
	ATOM	2324		S 54	37.645	11.206	34.448	1.00 28.56	s
	ATOM	-2325	OH2 TIP	S 55	26.371	28.513	12.142	1.00 32.08	S
	ATOM	2326	OH2 TIP	S 58	33.564	19.700	3.483	1.00 28.28	s
	ATOM	2327	OH2 TIP	S 64	48.295	-0.632	14.280	1.00 32.13	S
15	ATOM	2328	OH2 TIP	S 65	40.064	26.036	34.324	1.00 24.17	s
	MOTA	2329	OH2 TIP	S 66	29.570	3.958	14.729	1.00 28.94	S
	MOTA	2330	OH2 TIP	S 72	60.085	11.604	6.814	1.00 38.35	S
	ATOM	2331	OH2 TIP		39.203	44.403	18.686	1.00 26.61	s
	ATOM	2332	OH2 TIP		47.312	12.366	27.366	1.00 28.51	S
20	ATOM	2333		S 80	43.862	33.771	33.329	1.00 28.82	S
20	ATOM	2334		S 81	57.890	13.106	2.128	1.00 20.62	S
	ATOM	2335	OH2 TIP		41.663	34.381	32.043	1.00 40.62	
									S
	ATOM	2336		S 85	50.974	40.331	19.200	1.00 21.14	S
0.5	ATOM	2337		S 88	47.925	-0.832	-6.556	1.00 24.11	S
25	ATOM	2338	OH2 TIP		27.231	28.336	33.481	1.00 27.64	S
	MOTA	2339		s 91	43.651	-7.101	-7.995	1.00 24.33	S
	ATOM	2340	OH2 TIP		49.325	4.387	19.370	1.00 28.02	S
	MOTA	2341	OH2 TIP	s 93	46.231	11.549	33.898	1.00 29.40	S
	MOTA	2342	OH2 TIP	5 94	63.889	24.831	1.168	1.00 26.53	S
30	ATOM	2343	OH2 TIP	s 96	56.396	4.952	-6.749	1.00 28.00	S
	ATOM	2344	OH2 TIP	s 98	35.510	27.986	11.558	1.00 29.24	S
	ATOM	2345	OH2 TIP	5 100	49.942	24.366	30.265	1.00 31.61	S
	ATOM	2346	OH2 TIP	s 101	56.121	7.113	-8.298	1.00 31.57	S
	ATOM	2347	OH2 TIP	S 102	58.318	19.957	-8.378	1.00 26.95	S
35	ATOM	2348	OH2 TIP		49.647	22.446	39.624	1.00 40.57	S
	ATOM	2349	OH2 TIP		45.359	7.052	13.052	1.00 26.27	S
	ATOM	2350	OH2 TIP		37.150	32.340	32.346	1.00 34.45	S
	ATOM	2351	OH2 TIP		43.465	40.457	8.240	1.00 40.48	s
	ATOM	2352	OH2 TIP		36.644		13.418	1.00 30.70	S
40	ATOM	2353	OH2 TIP		41.912	-8.974	-8.264	1.00 26.08	s
70	ATOM	2354	OH2 TIP		62.424	15.800	-7.411	1.00 24.08	S
	ATOM	2355	OH2 TIP		37.266	18.656	-9.097	1.00 24.00	S
		2356						1.00 25.19	
	ATOM		OH2 TIP		43.129	26.845	14.606		S
4.5	ATOM	2357	OH2 TIP		36.339	32.639	29.802	1.00 29.25	S
45	MOTA	2358	OH2 TIP		54.051		26.498	1.00 33.93	S
	ATOM	2359	OH2 TIP				5.492	1.00 33.72	S
	MOTA	2360	OH2 TIP		38.873	25.163	36.697	1.00 30.69	s
	ATOM	2361	OH2 TIP			8.553	25.307	1.00 31.43	S
	ATOM	2362	OH2 TIP S	3 135	53.672	10.546		1.00 33.45	S
50	ATOM	2363	OH2 TIP S	136	59.892	15.434	11.467	1.00 31.39	S
	ATOM	2364	OH2 TIP S	137	31.040	12.361	35.470	1.00 34.07	S
	ATOM	2365	OH2 TIP S	3 139	33.489	14.292	-0.598	1.00 40.68	S
	ATOM	2366	OH2 TIP S		46.918	8.748	11.662	1.00 29.23	s
	ATOM	2367	OH2 TIP S		46.297	-7.287	-9.196	1.00 42.20	S
55	ATOM	2368	OH2 TIP		58.193	6.715	-4.685	1.00 35.48	s
	ATOM	2369	OH2 TIP		44.598	4.435	12.503	1.00 27.68	S
	ATOM	2370	OH2 TIP S			5.999	12.450	1.00 27.00	S
	ATOM	2371	OH2 TIP S		43.676	32.852	35.735	1.00 35.70	S
	ATOM	2372	OH2 TIP S		35.783		36.452	1.00 33.70	S
	WION	231.2	OHZ IIF	. T40	33.703	18.628	30.432	1.00 34.02	3

	ATOM	2373	OH2 TIP S	147	25.402	4.058	20.638	1.00 45.03	s
	ATOM	2374	OH2 TIP S		45.839	35.853	33.724	1.00 35.47	S
	ATOM	2375	OH2 TIP S	149	22.176	18.976	16.752	1.00 31.87	s
	MOTA .	2376	OH2 TIP S	150	43.986	33.179	10.162	1.00 37.70	S
5	MOTA	2377	OH2 TIP S	151	50.653	20.347	42.428	1.00 35.80	S
	ATOM	2378	OH2 TIP S	152	47.843	24.314	9.506	1.00 31.05	S
	ATOM	2379	OH2 TIP S	153	44.693	5.273	-14.175	1.00 29.90	S
	ATOM	2380	OH2 TIP S	155	26.560	36.851	31.684	1.00 49.29	S
	ATOM	2381	OH2 TIP S	156	46.867	8.019		1.00 29.21	S
10	MOTA	2382	OH2 TIP S	157	30.432	28.741	12.438	1.00 37.76	S
	ATOM	2383	OH2 TIP S	158	41.004	20.553	6.423	1.00 39.53	s
	ATOM	. 2384	OH2 TIP S	159	49.258	20.069	29.294	1.00 33.97	S
	ATOM	2385	OH2 TIP S	160	48.082	28.459	16.489	1.00 33.10	S
	ATOM	2386	OH2 TIP S	161	47.448	18.625	27.683	1.00 34.87	S
15	ATOM	2387	OH2 TIP S	162	19.687	20.632	23.411	1.00 35.01	S
	ATOM	2388	OH2 TIP S	163	32.402	-1.266	22.443	1.00 37.26	S
	ATOM	2389	OH2 TIP S	164	39.475	33.468	33.237	1:00 35.34	S
	ATOM	2390	OH2 TIP S	165	44.277	18.950	5.162	1.00 45.14	S
	MOTA	2391	OH2 TIP S	166	34.797	30.523	10.736	1.00 47.55	S
20	MOTA	2392	OH2 TIP S	167	46.541	3.526	-14.949	1.00 26.54	S
	ATOM	2393	OH2 TIP S	168	36:333	16.371	1.539	1.00 38.68	s
	ATOM	2394		169	46.761	38.936	27.403	1.00 34.66	S
	MOTA	2395	OH2 TIP S	170	24.163	13,.264	11.375	1.00 41.23	S
	MOTA	2396		171	48.459	15.018	31.951	1.00 38.11	S
25	MOTA	2397		172	34.261	23.193	40.004	1.00 48.96	· S
	ATOM	2398		173	45.924	-0.026	13.224	1.00 39.55	S
	MOTA	2399		175	41.384	37.389	32.543	1.00 40.74	S
	MOTA	2400		177	49.394	35.312	27.150	1.00 44.33	S
	MOTA	2401		178	29.066	29.942	34.359	1.00 41.46	S
30	MOTA	2402		180	49.354	19.467	7.273	1.00 34.56	S
	ATOM	2403		181	25.298	17.029	31.863	1.00 47.74	S
	ATOM	2404		182	37.071	25.027	4.669	1.00 43.87	S
	ATOM	2405	OH2 TIP S	183	22.581	7.487	18.691	1.00 41.75	S
25	ATOM	2406	OH2 TIP S	184	32.269	7.011	-1.891	1.00 48.84	S
35	ATOM	2407		185	48.234	0.494	6.833	1.00 48.16	S
	ATOM	2408	OH2 TIP S	187	20.008	14.658	19.211	1.00 45.27	S
	MOTA	2409	OH2 TIP S	188	49.341	22.698	42.272	1.00 42.20	S
	ATOM	2410 2411		190	61.292	18.260 10.606	-8.097	1.00 45.21	S
40	ATOM ATOM	2411		191 192	28.152 25.626		2.819	1.00 40.38	S
40	ATOM	2412		192	59.876	12.619	23.191 1.216	1.00 34.27 1.00 46.54	s s
	ATOM	2413		194	57.592	11.603	-10.646	1.00 45.82	S
	ATOM	2414	OH2 TIP S	195	31.509	36.649	21.499	1.00 45.82	S
	ATOM	2416	OH2 TIP S		50.270	-1.543	-6.136	1.00 42.66	S
45	ATOM	2417	OH2 TIP S		24.467	8.729	13.088	1.00 42.78	S
	ATOM	2418	OH2 TIP S		38.098	8.699	25.759	1.00 32.80	S
	ATOM	2419	OH2 TIP S		57.831		-13.255	1.00 32.30	S
	ATOM	. 2420	OH2 TIP S		23.888	22.328	30.524	1.00 43.31	S
	ATOM	2421	OH2 TIP S		47.691	26.068	37.666	1.00 37.12	S
50	ATOM	2422	OH2 TIP S		38.653	7.070	29.307	1.00 50.54	s
	ATOM	2423	OH2 TIP S		44.424	27.583	2.092	1.00 53.50	S
	ATOM	2424	OH2 TIP S		22.258	2.296	17.948	1.00 47.38	s
	ATOM	2425	OH2 TIP S		19.843	17.943	23.303	1.00 30.36	s
	ATOM	2426	OH2 TIP S		27.647	11.344	24.681	1.00 31.32	S
55	ATOM	2427	OH2 TIP S		37.953	7.817	-9.284	1.00 45.97	Š
	ATOM	2428	OH2 TIP S		33.845	34.040	12.124	1.00 38.11	s
	ATOM	2429	OH2 TIP S		58.484	15.269	13.717	1.00 38.26	S
	ATOM	2430	OH2 TIP S		48.526	40.920	26.583	1.00 35.23	S
	ATOM	2431	OH2 TIP S		52.094	21.184	38.122	1.00 29.86	S
			9						~

	MOTA	2432	OH2 TIP S 223	36.889	5.881	3.281	1.00 37.63	S
	ATOM	2433	OH2 TIP S 224	47.642	•	-10.684	1.00 34.89	S
	ATOM	2434	OH2 TIP S 226	47.284	2.916	19.133	1.00 34.10	S
	ATOM	2435	OH2 TIP S 227	42.468		-15.039	1.00 37.98	S
5	ATOM	2436	OH2 TIP S 228	19.169	22.832	21.831	1.00 41.57	S
	ATOM	2437	OH2 TIP S 231	57.592	12.689	14.880	1.00 50.22	S
	ATOM	2438	OH2 TIP S 232	27.102	9.176	5.655	1.00 30.22	S
	ATOM	2439	OH2 TIP S 233	58.618		-11.925	1.00 40.37	S
	ATOM	2440	OH2 TIP S 234	22.822	25.342	19.945	1.00 30.71	S
10	ATOM	2441	OH2 TIP S 236	24.831	32.218	28.901	1.00 34.93	S
- •	ATOM	2442	OH2 TIP S 237	20.045	10.774	16.992	1.00 37.69	
	ATOM	2443	OH2 TIP S 238		19.850	15.679	1.00 39.57	s s
	ATOM	2444	OH2 TIP S 239	19.490	20.949	26.114		
	ATOM	2445	OH2 TIP S 240	61.187	26.377	7.346	1.00 34.55	. S
15	ATOM	2446	OH2 TIP S 241	33.680	38.342	19.389	1.00 39.66	S
12	ATOM	2447	OH2 TIP S 241	51.539	31.612	10.881	1.00 48.93	S
	ATOM	2448	OH2 TIP S 244	25.872	14.431	30.404		S
	ATOM	2449	OH2 TIP S 244 OH2 TIP S 248	37.332	5.849	9.544	1.00 46.69 1.00 43.81	
	ATOM	2450	OH2 TIP S 250	39.087	-1.293	-9.655		S
20	ATOM	2451	OH2 TIP S 258	23.938	30.000	30.010	1.00 42.96	S
20	ATOM	2452	OH2 TIP S 259	24.949		32.578	1.00 38.89 1.00 40.17	s
	ATOM	2453	OH2 TIP S 259	32.111	29.749			S
	ATOM	2453	OH2 TIP S 266	21.404	17.986	1.918	1.00 48.36	s
	ATOM	2455	OH2 TIP S 269	35.425	12.876 36.767	25.603	1.00 57.17	S
25	ATOM	2456	OH2 TIP S 209	52.438	25.529	12.550 30.131	1.00 30.70 1.00 44.85	s s
23	ATOM	2457		53.299	20.156	36.003	1.00 44.85	S
	ATOM	2458	OH2 TIP S 272	50.914	6.919	23.723	1.00 37.15	S
	ATOM	2459	OH2 TIP S 274	31.578	30.795	11.014	1.00 43.29	S
	ATOM	2460	OH2 TIP S 275	26.341	7.243	22.447	1.00 30.13	S
30	ATOM	2461	OH2 TIP S 276	60.392	18.195	10.235	1.00 33.40	S
	ATOM	2462	OH2 TIP S 277	47.355	-9.081		1.00 37.91	s
	ATOM	2463	OH2 TIP S 279	41.304		-16.647	1.00 38.12	S
	ATOM	2464	OH2 TIP S 282	33.299	21.620	37.881	1.00 36.12	S
	ATOM	2465	OH2 TIP S 283	56.469	26.112	-8.575	1.00 43.71	S
35	ATOM	2466	OH2 TIP S 287		26.573	7.246	1.00 41.43	s
	ATOM	2467	OH2 TIP S 288	56.240		-11.331	1.00 41.79	S
	ATOM	2468	OH2 TIP S 290	49.060	14.978	28.166	1.00 37.03	s
	ATOM	2469	OH2 TIP S 291	37.095	44.270	26.442	1.00 45.08	S
	ATOM	2470	OH2 TIP S 292	47.814	-0.384		1.00 48.60	S
40	ATOM	2471	OH2 TIP S 297	58.081	2.784	-7.841	1.00 41.89	s
	ATOM	2472	OH2 TIP S 298	36.447	45.321	18.644	1.00 54.91	s
	ATOM	2473	OH2 TIP.S 299	49.029	23.328	1.767	1.00 30.55	s
	ATOM	2474	OH2 TIP S 301	24.375	13.771	8.634	1.00 48.47	s
	ATOM	2475	OH2 TIP S 303	47.904	36.798	28.653	1.00 35.76	S
45	ATOM	2476	OH2 TIP S 305	51.156	40.821	27.172	1.00 43.59	S
	ATOM	2477	OH2 TIP S 306	32.943	28.917	35.227	1.00 42.60	S
	ATOM	2478	OH2 TIP S 307	58.462	28.373	6.251	1.00 46.15	S
	ATOM	2479	OH2 TIP S 308	41.964	30.940	36.712	1.00 48.26	S
	ATOM	2480	OH2 TIP S 313	51.176	-1.922	-3.336	1.00 50.61	S
50	MOTA	2481	OH2 TIP S1001	21.319	36.868	23.805	1.00 36.97	s
	MOTA	2482	OH2 TIP S1002	48.880	32.620	27.617	1.00 44.40	S
	MOTA	2483	OH2 TIP S1003	61.880	19.473	11.767	1.00 45.49	S
	ATOM	2484	OH2 TIP S1004	52.770	21.424	26.815	1.00 24.43	s
	MOTA	2485	OH2 TIP S1005	35.373	29.094	36.197	1.00 35.97	S
55	MOTA	2486	OH2 TIP S1006	40.815	-6.636	4.389	1.00 43.15	S
	MOTA	2487	OH2 TIP S1007	44.953	1.286	11.272	1.00 49.45	S
	ATOM	2488	OH2 TIP S1010	21.004	16.168	27.009	1.00 48.51	S
	ATOM	2489	OH2 TIP S1011	47.094	41.786	9.243	1.00 50.10	S
	ATOM	2490	OH2 TIP S1012	32.479	2.978	14.158	1.00 49.47	S

	ATOM	2491	012 GLC	G	1		48.557	11.372	-12.279	1.00 40.72	. G
	MOTA	2492	C11 GLC	G	1		48.836	12.133	-11.097	1.00 38.05	
	MOTA	2493	C13 GLC	G	1		49.266	13.554	-11.476	1.00 38.09	
	ATOM	2494	014 GLC	G	1	•	49.559	14.299	-10.292	1.00 33.99	
5	ATOM	2495	C15 GLC	G	1		48.150		-12.257	1.00 37.32	: G
	ATOM	2496	016 GLC	G	1		48.574		-12.604	1.00 36.74	
	ATOM	2497	012 GLC		2		40.114	-6.634	-6.562	1.00 33.52	
	ATOM	2498	C11 GLC		2		38.967	-6.592	-7.404	1.00 31.05	
	ATOM	2499	C13 GLC		2		37.712	-6.417	-6.552	1.00 31.56	
10	ATOM	2500	014 GLC		2		36.554	-6.406		1.00 30.70	
~ ~	ATOM	2501	C15 GLC		2		37.792	-5.109		1.00 30.03	
	ATOM	2502	016 GLC		2		36.609	-4.961	-4.975	1.00 29.66	
	ATOM	2502	010 GLC		3		44.030		-13.470	1.00 23.00	
	ATOM	2504	C11 GLC		3		43.950		-13.690	1.00 37.90	
15	ATOM	2505	C11 GLC		3		42.747		-14.579	1.00 38.47	
13		2505	O14 GLC		3		41.551		-14.379	1.00 39.32	
	ATOM		C15 GLC		3		42.878		-15.942	1.00 39.39	
	ATOM	2507									
	ATOM	2508	016 GLC		3		41.736		-16.731	1.00 40.78	
00	MOTA	2509	012 GLC		5		40.556	1.005	2.289	1.00 45.25	
20	ATOM	2510	C11 GLC		5		40.966	2.332	1.960	1.00 40.56	
	ATOM	2511	C13 GLC		5		40.187	3.327	2.814	1.00 40.36	
	ATOM	2512	O14 GLC		5		38.791	3.169	2.572	1.00 40.71	
	ATOM	2513	C15 GLC		5		40.619	4.751	2.464	1.00 40.04	
	ATOM	2514	016 GLC		5		39.885	5.681	3.256	1.00 36.89	•
25	MOTA	2515	O12 GLC		6		36.951	22.702	40.046	1.00 63.04	
	MOTA	2516	C11 GLC		6		37.592	21.583	39.422	1.00 62.46	
	ATOM	2517	C13 GLC		6		38.104	21.978	38.030	1.00 61.14	
	MOTA	2518	O14 GLC		6		39.034	23.054	38.168	1.00 61.72	
	ATOM	2519	C15 GLC		6		36.948	22.429	37.126	1.00 60.51	
30	ATOM	2520	O16 GLC		6		35.992	21.372	36.960	1.00 58.61	
	MOTA	2521	O12 GLC		7		37.316	0.281	14.299	1.00 73.45	
	MOTA	2522	C11 GLC		7		37.655	-0.758	15.222	1.00 72.78	
	ATOM	2523	C13 GLC		7		36.592	-1.856	15.157	1.00 72.98	
	ATOM	2524	O14 GLC		7		35.320	-1.299	15.498	1.00 73.88	
35	MOTA	2525	C15 GLC		7		36.924	-2.989	16.134	1.00 73.66	
	MOTA	2526	O16 GLC		7		36.972	-2.493	17.478	1.00 75.38	
	MOTA	2527	O12 GLC		8		51.921	21.898	5.908	1.00 62.51	
	ATOM	2528	C11 GLC		8		52.447	20.871	5.063	1.00 63.42	
	ATOM	2529	C13 GLC		. 8		51.47.6	20.597	3.908	1.00 64.28	
40	ATOM	2530	O14 GLC		8		51.297	21.794	3.150	1.00 66.28	
	MOTA	2531	C15 GLC		8		50.121	20.137	4.448	1.00 64.49	
	ATOM	2532	O16 GLC		8		49.233	19.886	3.357	1.00 64.01	
	MOTA	2533	O12 GLC		10		36.044	37.499	29.523	1.00 56.89	
	MOTA	2534	C11 GLC		10		35.164	36.645	30.259	1.00 56.97	
45	ATOM	2535	C13 GLC		10		33.849	36.489	29.494	1.00 56.11	
	MOTA	2536	O14 GLC		10		33.248	37.772	29.308	1.00 56.44	
	ATOM	2537	C15 GLC				32.900	35.580	30.277	1.00 55.84	
	MOTA	2538	O16 GLC		10		31.674	35.442	29.557	1.00 55.39	
	ATOM	2539	O3G ATP	N	1		46.280	25.658	5.170	1.00 51.49	
50	ATOM	2540	PG ATP		1		46.464	25.053	3.691	1.00 52.22	
	MOTA	2541	O1G ATP	N	1		47.406	23.911	3.763	1.00 51.41	
	MOTA	2542	O2G ATP	N	1		46.794	26.182	2.784	1.00 52.07	
	MOTA	2543	O3B ATP	N.	1		44.976	24.513	3.344	1.00 51.01	
	ATOM	2544	PB ATP		1		44.560	22.969	3.605	1.00 50.20	
55	MOTA	2545	O1B ATP		1		43.083	22.898	3.669	1.00 49.41	
	MOTA	2546	O2B ATP		1		45.345	22.474	4.766	1.00 50.34	
	ATOM	2547	O3A ATP	N	1		45.070	22.231	2.255	1.00 47.77	
	ATOM	2548	PA ATP		1		45.075	20.613	2.121	1.00 42.84	
•	ATOM	2549	O1A ATP	N	1		45.547	20.291	0.754	1.00 43.81	N

	ATOM	2550		ATP				45.807	20.035	3.270	1.00	45.03	N
	ATOM	2551		ATP				43.516	20.223	2.245	1.00	41.73	N .
	MOTA	2552		ATP				42.528	20.925	1.489	1.00	37.57	N
	ATOM	2553	C4*	ATP	N	1		41.127	20.379	1.776	1.00	39.45	N
5	MOTA	2554	04*	ATP	N	1		40.907	19.024	1.279	1.00	37.72	N
	ATOM	2555	C3*	ATP	N	1		40.777	20.321			38.48	N
	ATOM	2556	03*					40.360	21.615		1.00		N
	ATOM	2557	C2*				•	39.608	19.374	3.270		37.58	N
	ATOM	2558	02*			ī		38.410	20.076			35.98	N
10	MOTA	2559	C1*			1		39.939	18.346			35.55	N
	ATOM	2560	N9	ATP		ī		40.628	17.156			31.76	N
	ATOM	2561	C8	ATP		ī		41.864	17.126			30.49	N
	ATOM	2562	N7	ATP		1		42.143	15.877	3.667		29.75	N
	ATOM	2563	C5	ATP		1		41.088	15.118	3.390		27.49	
15	ATOM	2564	C4	ATP		1		40.125					N
13									15.925	2.810	1.00	30.02	N
	MOTA	2565	N3 C2	ATP		1		38.937	15.389	2.431		27.11	N
	ATOM	2566		ATP		1		38.679	14.085	2.615		25.62	N
	ATOM	2567	N1	ATP		1		39.597	13.283	3.175		21.76	N
	MOTA	2568	C6	ATP		1		40.800	13.768	3.571		23.90	N
20	ATOM	2569	N6	ATP		1		41.698	12.964	4.127	1.00		N
	ATOM	2570	S	SO4		1		58.680	8.493	-0.639		56.05	I
	ATOM	2571	01	SO4		1		57.956	7.875	0.483		58.83	. I
	ATOM	2572	02	SO4		1		57.886	9.607	-1.188		57.04	I
	ATOM	2573	03	SO4		1		58.906	7.478	-1.683		57.47	I
25	MOTA	2574	04	SO4	I	1		59.976	9.008	-0.156	1.00	57.51	, I
	MOTA	2575	S	SO4		2		39.339	4.855	7.057	1.00	84.24	I
	ATOM	2576	01	SO4	I	2		39.390	6.175	7.711	1.00	85.02	I
	MOTA	2577	02	SO4	Ι	2		40.101	4.897	5.797	1.00	84.75	I
	MOTA	2578	03	SO4	I	2		37.936	4.506	6.766	1.00	84.94	I
30	ATOM	2579	04	SO4	I	2		39.931	3.842	7.954	1.00	84.44	I
	ATOM	2580	S	SO4	I	3		38.987	-2.256	3.310	1.00	58.58	I
	ATOM	2581	01	SO4	I	3		37.734	-1.675	3.827	1.00	59.11	I
	ATOM	2582	02	SO4	I	3		39.460	-1.454	2.172	1.00	59.91	I
	ATOM	2583	03	SO4	I	3		38.743	-3.640	2.866	1.00	60.97	I
35	ATOM	2584	04	SO4	I	3		40.014	-2.260	4.369	1.00	59.58	I
	ATOM	2585	S	SO4	I	4		34.397	5.289	30.981	1.00	64.34	I
	ATOM	2586	01	SO4	I	4		33.627	6.528	30.742	1.00	60.43	I
	ATOM	2587	02	SO4	I	4		34.337	4.427	29.782		60.11	I
	ATOM	2588	03	SO4	I	4		33.816	4.572	32.133	1.00	64.39	. I
40	ATOM	2589	04	SO4	I	4		35.806	5.626	31.277		63.55	I
	ATOM	2590	S	SO4	I	5		55.074	-6.984	-3.711		75.40	Ī,
	ATOM	2591	01	SO4	I	5		54.657	-7.518	-2.399		74.66	Ī
	ATOM	2592	02	SO4	I	5		54.209	-5.845	-4.065		74.96	Ī
	ATOM	2593	03	504		5		54.950	-8.034	-4.742		74.22	ī
45	ATOM	2594	04	SO4		5		56.477	-6.532	-3.633		75.15	ī
	ATOM	2595	02	PO4				57.362	24.998	13.149		66.76	P
	ATOM	2596	03	PO4				59.399	26.166	13.761		66.89	. P
	ATOM	2597	04	PO4				57.761	25.606	15.462		67.43	P
	ATOM	2598		PO4								65.91	
50			01	PO4				57.264	27.325 26.025	13.818			P P
50	ATOM	2599	P		P			57.947		14.048		66.69	
	ATOM	2600	CB	GLU		80		50.411		-13.538		23.31	AC2
•	ATOM	2601	CG	GLU		80		51.306		-14.362		24.09	AC2
	ATOM	2602	CD	GLU		80		52.180		-13.509		25.31	AC2
	ATOM	2603		GLU		80		52.841		-12.580		22.80	AC2
55	ATOM	2604		GLU		80		52.212		-13.774		28.07	AC2
	MOTA	2605	CB	SER		105		37.582	-1.281	-6.192		21.16	AC2
	ATOM	2606	OG	SER		105		37.127	-1.871	-4.988		20.42	AC2
	ATOM	2607	CB	ARG		116		59.520	22.977	-7.867		31.00	AC2
	ATOM	2608	CG	ARG		116		60.312	24.192	-8.323	0.50	32.50	AC2

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ATOM
             2609 CD
                        ARG
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                                                                    0.50 34.11
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      MOTA
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                                                                          8.20
                                                                                      AC2
     MOTA
             2617
                    CD2 LEU
                               145
                                         52.030
                                                   9.361
                                                            6.087
                                                                    0.50 10.66
                                                                                      AC2
     MOTA
             2618
                    CB
                        ARG
                               183
                                       . 27.455
                                                  16.155
                                                           24.989
                                                                    0.50 19.21
                                                                                      AC2
     MOTA
             2619
                    CG
                        ARG
                               183
                                         28.077
                                                  15.397
                                                           26.147
                                                                    0.50 18.46
                                                                                      AC2
     ATOM
             2620
                    CD
                        ARG
                               183
                                         27.002
                                                  14.945
                                                           27.127
                                                                    0.50 19.72
                                                                                      AC2
     ATOM
             2621
                   NE
                        ARG
                               183
                                         26.016
                                                  14.086
                                                           26.478
                                                                    0.50 18.79
                                                                                      AC2
     MOTA
             2622
                    CZ
                        ARG
                               183
                                         24.703
                                                  14.279
                                                           26.539
                                                                    0.50 18.52
                                                                                      AC2
15
     ATOM
             2623
                   NH1 ARG
                               183
                                         24.213
                                                  15.305
                                                           27.221
                                                                    0.50 15.35
                                                                                      AC2
     ATOM
             2624
                   NH2 ARG
                               183
                                         23.881
                                                  13.445
                                                           25.915
                                                                    0.50 17.55
                                                                                      AC2
     MOTA
             2625
                   CB
                        SER
                               191
                                         38.479
                                                  10.847
                                                           23.036
                                                                    0.50 16.57
                                                                                      AC2
     MOTA
             2626
                        SER
                   OG
                               191
                                         37.418
                                                  10.765
                                                           23.973 , 0.50 18.62
                                                                                      AC2
     MOTA
             2627
                   CB
                        GLU
                               209
                                         38.645
                                                  24.079
                                                            8.551
                                                                    0.50 22.02
                                                                                     AC2
20
     ATOM
             2628
                        GLU
                   CG
                               209
                                         37.769
                                                  25.296
                                                            8.263
                                                                    0.50 23.40
                                                                                      AC2
     ATOM
             2629
                   CD
                        GLU
                               209
                                         37.513
                                                  26.175
                                                            9.483
                                                                    0.50 24.27
                                                                                      AC2
             2630
     MOTA
                   OE1
                       GLU
                               209
                                         37.076
                                                  27.328
                                                            9.288
                                                                    0.50 25.25
                                                                                     AC2
     MOTA
             2631
                   OE2
                       GLU
                               209
                                         37.737
                                                  25.727
                                                           10.629
                                                                   0.50 20.24
                                                                                     AC2
     MOTA
             2632
                   CB
                        GLN
                               247
                                         38.598
                                                  32.546
                                                          14.790
                                                                    0.50 18.71
                                                                                     AC2
25
     MOTA
             2633
                   CG
                        GLN
                               247
                                         38.077
                                                  33.665
                                                           13.900
                                                                   0.50 16.95
                                                                                     AC2
     MOTA
             2634
                   CD
                        GLN
                               247
                                         38.614
                                                  33.598
                                                          12.479
                                                                   0.50 19.13
                                                                                     AC2
     MOTA
                                         39.763
             2635
                   OE1 GLN
                               247
                                                  33.221
                                                          12.246
                                                                   0.50 17.24
                                                                                     AC2
     ATOM
             2636
                   NE2
                       GLN
                               247
                                         37.780
                                                  33.979
                                                          11.520
                                                                   0.50 19.88
                                                                                     AC2
     ATOM
             2637
                   CE
                        LYS
                               315
                                         34.978
                                                  25.150
                                                          36.369
                                                                   0.50 20.49
                                                                                     AC2
     ATOM
             2638
                   ΝZ
                        LYS
                               315
                                         34.183
                                                  24.074
                                                          37.023
                                                                   0.50 17.05
                                                                                     AC2
     ATOM
             2639
                   CB
                        GLN
                               352
                                         32.365
                                                  1.170
                                                          19.731
                                                                   0.50 31.10
                                                                                     AC2
     MOTA
             2640
                   CG
                        GLN
                               352
                                         33.833
                                                   0.778
                                                          19.683
                                                                   0.50 32.11
                                                                                     AC2
     ATOM
             2641
                   CD
                        GLN
                               352
                                         34.190
                                                   0.027
                                                          18.419
                                                                   0.50 33.04
                                                                                     AC2
     ATOM
             2642
                   OE1 GLN
                               352
                                         33.906
                                                  0.485
                                                          17.314
                                                                   0.50 34.87
                                                                                     AC2
35
     MOTA
             2643
                   NE2 GLN
                              352
                                         34.819
                                                 -1.133
                                                          18.575
                                                                   0.50 32.08
                                                                                     AC2
     END
```

Example 3: Co-ordinates for the PDK1 fragment without alternate side chains.

40

```
REMARK coordinates from restrained individual B-factor refinement
    REMARK refinement resolution: 25.0 - 2.0 A
    REMARK starting r= 0.1972 free_r= 0.2220
    REMARK final
                    r= 0.1954 free r= 0.2224
    REMARK B rmsd for bonded mainchain atoms=
45
                                               1.501
                                                       target= 1.5
    REMARK B rmsd for bonded sidechain atoms= 2.235
                                                      target= 2.0
    REMARK B rmsd for angle mainchain atoms= 2.347
                                                      target= 2.0
    REMARK B rmsd for angle sidechain atoms=
                                              3.302
    REMARK rweight= 0.0900 (with wa= 1.29263)
50
    REMARK target= mlf steps= 30
    REMARK sg= P3(2)21 a= 123.013 b= 123.013 c= 47.624 alpha= 90 beta= 90
    gamma= 120
    REMARK parameter file 1
                             : /ddl/david/projects/PDK1 new/CNS/prot.par
    REMARK parameter file 2
                             : /ddl/david/projects/PDK1_new/CNS/atp.par
55
    REMARK parameter file 3
                             : CNS_TOPPAR:water_rep.param
    REMARK parameter file 4
                             : CNS_TOPPAR:ion.param
```

```
REMARK parameter file 5 : /ddl/david/projects/PDKl_new/CNS/glycerol.par
     REMARK molecular structure file: ../generate/alternate.mtf
     REMARK input coordinates: ../minimize/minimize.pdb
     REMARK reflection file= ../../1/hkl/cns.hkl
     REMARK ncs= none
     REMARK B-correction resolution: 6.0 - 2.0
     REMARK initial B-factor correction applied to fobs :
     REMARK
               B11= -2.766 B22= -2.766 B33=
                                                 5.532
               B12= -0.375 B13=
     REMARK
                                  0.000 B23=
                                                 0.000
10
     REMARK B-factor correction applied to coordinate array B:
     REMARK bulk solvent: density level= 0.378441 e/A^3, B-factor= 52.6885 A^2
     REMARK reflections with |Fobs|/sigma F < 0.0 rejected.
     REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
     REMARK theoretical total number of refl. in resol. range:
                                                                      28210 ( 100.0
15
     육 )
     REMARK number of unobserved reflections (no entry or |F|=0):
                                                                        568 (
                                                                                 2.0
     ୫ )
     REMARK number of reflections rejected:
                                                                          0 (
                                                                                 0.0
20
     REMARK total number of reflections used:
                                                                      27642 (
                                                                               98.0
     REMARK number of reflections in working set:
                                                                      27063 (
                                                                               95.9
     REMARK number of reflections in test set:
                                                                        579 ( - 2.1
25
     ક )
     CRYST1 123.013 123.013
                                47.624 90.00 90.00 120.00 P 32 2 1
     REMARK FILENAME="bindividual.pdb"
     REMARK DATE:16-Apr-2002 18:31:12
                                              created by user: david
     REMARK VERSION:1.0
.30
     ATOM
                             71
               1 CB PRO A
                                      58.912 -7.251
                                                        8.216
                                                               1.00 67.78
     MOTA
               2
                  CG PRO A
                              71
                                      59.621
                                              -6.941
                                                        9.534
                                                               1.00 69.16
                                                                               Α
     MOTA
               3
                  С
                       PRO A
                             71
                                      59.493
                                              -6.506
                                                        5.894
                                                               1.00 67.06
     ATOM
               4
                       PRO A
                  0
                             71
                                      59.196
                                              -5.318
                                                        5.766
                                                               1.00 66.66
               5
     ATOM
                  N
                       PRO A
                                      60.984
                                              -6.073
                             71
                                                        7.833
                                                               1.00 67.86
                                                                                Α
35
                                                        9.207
     MOTA
               6
                  CD
                       PRO A
                              71
                                      60.554
                                              -5.762
                                                               1.00 68.24
                                                                               Α
     MOTA
               7 .
                  CA
                       PRO A
                              71
                                      60.040
                                              -7.035
                                                        7.217
                                                               1.00 67.75
                                                                               Α
     MOTA
               8
                  N
                       PRO A
                              72
                                      59.356
                                              -7.385
                                                        4.890
                                                               1.00 66.32
                                                                               Α
                             72
     MOTA
               9
                                      59.712
                                              -8.816
                  CD
                       PRO A
                                                        4.898
                                                               1.00 67.17
                                                                               Α
     ATOM
              10
                       PRO A
                                      58.840
                                              -6.986
                  CA
                              72
                                                        3.578
                                                               1.00 65.61
                                                                               Α
     ATOM
              11
                  CB
                       PRO A
                             .72
                                      58.672
                                              -8.321
                                                        2.858
                                                               1.00 66.47
                                                                               Α
     MOTA
              12
                              72
                                      59.796
                                              -9.133
                  CG
                      PRO A
                                                        3.419
                                                               1.00 67.57
                                                                               A
              13
     ATOM
                  С
                       PRO A
                              72
                                      57.527
                                              -6.208
                                                        3.673
                                                               1.00 63.94
                                                                               Α
     MOTA
              14
                  0
                       PRO A
                              72
                                      56.710
                                              -6.451
                                                        4.561
                                                               1.00 64.11
                                                                               Α
     MOTA
              15
                  N
                      ALA A
                              73
                                      57.341
                                              -5.268
                                                       2.753
                                                               1.00 61.57
                                                                               Α
45
     ATOM
              16
                 · CA
                      ALA A
                              73
                                      56.133
                                              -4.454
                                                       2.708
                                                               1.00 58.74
                                                                               Α
     ATOM
              17
                  CB
                      ALA A
                              73
                                      56.438
                                              -3.030
                                                       3.165
                                                               1.00 58.05
                                                                               Α
     MOTA
              18
                  С
                      ALA A
                              73
                                      55.626
                                              -4.448
                                                       1.271
                                                               1.00 56.78
                                                                               Α
     ATOM
              19
                  0
                                      56.347
                      ALA A
                              73
                                              -4.834
                                                       0.349
                                                               1.00 56.95
                                                                               Α
     ATOM
              20
                  N
                      PRO A
                              74
                                      54.372
                                              -4.024
                                                       1.057
                                                               1.00 54.15
                                                                               Α
50
     ATOM
              21
                  CD
                      PRO A
                              74
                                      53.335
                                              -3.610
                                                       2.018
                                                              1.00 53.31
                                                                               A
     MOTA
              22
                  CA
                      PRO A
                              74
                                      53.856
                                              -4.003
                                                      -0.314
                                                              1.00 52.54
                                                                               Α
     ATOM
              23
                  CB
                      PRO A
                                              -3.375
                             74
                                      52.474
                                                      -0.148
                                                              1.00 52.86
                                                                               A
     MOTA
              24
                  CG
                      PRO A
                             74
                                      52.067
                                                              1.00 52.88
                                              -3.824
                                                       1.226
                                                                               Α
     ATOM
              25
                  С
                      PRO A
                              74
                                      54.772
                                              -3.167
                                                      -1.204
                                                               1.00 50.08
                                                                               Α
55
     ATOM
              26
                  0
                      PRO A
                              74
                                      55.559
                                              -2.361
                                                      -0.708
                                                               1.00 49.96
                                                                               Α
              27
                             75
                                      54.680
     ATOM
                  N
                      ALA A
                                              -3.366
                                                      -2.514
                                                               1.00 47.58
                                                                               Α
                             75
     ATOM
              28
                  CA
                      ALA A
                                      55.503
                                              -2.602
                                                      -3.446
                                                              1.00 44.69
                                                                               Α
     ATOM .
              29
                  CB
                      ALA A
                             75
                                                              1.00 46.14
                                      55.312
                                              -3.121
                                                      -4.870
                                                                               Α
     MOTA
              30
                             75
                      ALA A
                                      55.100
                                             -1.134
                                                      -3.371
                                                              1.00 41.55
                                                                               Α
```

	ATOM		31	0	·ALA	A	75		53.947	-0.813	-3.086	1.00 41.0	01	A
	MOTA		32	N.	LYS	A	76		56.053	-0.245	-3.619	1.00 38.3		A
	MOTA		33	CA	LYS	Α	76		55.781	1.184	-3.588	1.00 35.7		A
	MOTA		34	CB	LYS	A	76		57.053	1.957	-3.930	1.00 37.7		A
5	ATOM		35	CG	LYS	Α	76		57.123	3.356	-3.350	1.00 40.9		A
	ATOM		36	CD	LYS	A	76		57.262	3.316	-1.836	1.00 40.0) 4	Α
-	ATOM		37	CE	LYS	A	76		57.511	4.705	-1.277	1.00 42.0	8(A
	ATOM		38	NZ	LYS .	A	76		57.681	4.695	0.202	1.00 42.9	9	A
	MOTA	'	39	С	LYS .	Α	76		54.708	1.467	-4.638	1.00 32.6	55	A
10	ATOM		40	0	LYS .	A '	76	•	54.814	1.005	-5.770	1.00 31.4		A
	ATOM		41	N	LYS .	A '	77		53.668	2.207	-4.270	1.00 28.5		A
	ATOM		42	CA	LYS .	Α '	77		52.619	2.517	-5.232	1.00 25.7	2	A
	MOTA		43	CB	LYS .	A. '	77		51.316	2.865	-4.509	1.00 26.2		A
	ATOM		44	CG	LYS :	Α .	77		50.796	1.731	-3.631	1.00 27.1		A
15	MOTA		45	CD	LYS .	Α.	77		49.487	2.089	-2.967	1.00 26.8	0	A
	ATOM		46	CE	LYS		77		49.136	1.091	-1.870	1.00 27.3		A
	MOTA		47	NZ	LYS 2		77		48.998	-0.296	-2.380	1.00 27.1		Α,
	MOTA		48	С	LYS		77		53.053	3.668	-6.137	1.00 24.6		A
	ATOM		49	0	LYS	Α	77		54.010	4.377	-5.829	1.00 21.6		A
20	ATOM		50	N	ARG 2		78		52.351	3.838	-7.254	1.00 23.6		A
	MOTA		51	CA	ARG Z		78		52.662	4.897	-8.211	1.00 26.1		A.
	MOTA		52	СВ	ARG I		78		53.574	4.344	-9.318	1.00 28.5		· A
	ATOM		53	CG	ARG 2	Α.	78		53.017	3.139	-10.050	1.00 34.7		A
	ATOM		54	CD	ARG I		78		54.092	2.465	-10.896	1.00 40.9		A
25	MOTA		55	NE	ARG I		78		53.560	1.364		1.00 48.9		A
	ATOM		56	CZ	ARG 2		78		52.985		-11.203	1.00 52.5		A
	ATOM		57		ARG 2		78		52.860	0.113	-9.889	1.00 54.6		A
	ATOM		58		ARG 2		78		52.530	-0.672		1.00 54.0		A
	ATOM		59	С	ARG 2		78		51.382	5.488	-8.803	1.00 23.7		A
30	ATOM		60	ō	ARG Z		78		50.311	4.888	-8.706	1.00 24.2		A
	MOTA		61	N	PRO I		79		51.475	6.676	-9.428	1.00 21.7		A
	ATOM		62	CD	PRO I		79		52.691	7.475	-9.668	1.00 20.8		A
	ATOM		63	CA	PRO I		79		50.301		-10.021	1.00 21.9		A
	ATOM		64	СВ	PRO I		79		50.910		-10.816	1.00 22.2		A
35	ATOM	•	65	CG	PRO I		79		52.124		-10.014	1.00 22.1		Α
	ATOM		66	C ·	PRO Z		79		49.446		-10.903	1.00 22.8		A
	ATOM		67	Ō	PRO Z		79		48.213		-10.842	1.00 20.5		A
	ATOM		68	N	GLU Z		80		50.103		-11.714	1.00 21.8		A
	ATOM		69	CA	GLU Z		80		49,403		-12.628	1.00 22.9		A
40	ATOM		70	СВ	GLU Z		30		50.393		-13.571	1.00 25.2	4	A
	ATOM		71	CG	GLU I		30		51.230		-12.925	1.00 28.7		A
	ATOM		72	CD	GLU A		30		52.157		-13.913	1.00 31.9		A
	ATOM		73		GLU A		30		53.072		-14.433	1.00 34.3		A
•	ATOM		74		GLU A		30		51.969		-14.172	1.00 32.8		A
45	ATOM		75	C	GLU A	-	30		48.556		-11.912	1.00 22.0		A
	ATOM		76	Ö	GLU 2		30		47.692		-12.530	1.00 22.3		A
	ATOM		77	N	ASP A		31		48.804		-10.622	1.00 19.9		A
	ATOM		78	CA	ASP A		31		48.026	2.423	-9.874	1.00 19.9		A
	ATOM		79	СВ	ASP A		31		48.736	2.029	-8.571	1.00 21.1		A
50	ATOM		80	CG	ASP A		31		50.089	1.380	-8.807	1.00 22.4		A
	ATOM		81		ASP A		31		50.195	0.554	-9.731	1.00 24.2		A
	ATOM		82		ASP A		31		51.043	1.685	-8.058	1.00 23.3		A
	ATOM		83	C	ASP A		31		46.652	2.975	-9.518	1.00 20.8		A
	ATOM		84	0	ASP A		31		45.793	2.246	-9.015	1.00 20.0		A
55	ATOM		85	Ŋ	PHE A		32		46.445	4.258	-9.804	1.00 18.9		A
J.J	ATOM		86	CA	PHE A		32		45.200	4.934	-9.465	1.00 10.3		A
	ATOM		87	CB	PHE A		32		45.475	6.027	-8.427	1.00 19.3		Ā
	ATOM		88	CG	PHE A		32		46.134	5.531	-7.175	1.00 18.0		A
	ATOM		89		PHE A		32		45.371	5.136	-6.084	1.00 18.0		A
	MION		ひプ	CDT	CHD F	, 0	, 4.		40.01T	5.130	-0.004	T.OO T.1.T	•	A

								•			
	ATOM	90		PHE A	82	•	47.520	5.460	-7.086	1.00 18.99	Α
	MOTA .	91	CE1	PHE A	82	•	45.977	4.676	-4.918	1.00 17.12	· A
	MOTA	92	CE2	PHE A	82		48.137	5.000	-5.925	1.00 19.64	A
	ATOM	93	CZ	PHE A	82		47.361	4.607	-4.838	1.00 18.00	Α
5	ATOM	94	С	PHE A	82		44.476	5.596	-10.621	1.00 20.81	A
	MOTA	95	0	PHE A	82		45.066	5.933	-11.649	1.00 20.34	A
	ATOM	96	N	LYS A	83		43.182	5.792	-10.411	1.00 19.80	A
	ATOM	97	CA	LYS A	83		42.321	6.478	-11.353	1.00 21.65	A
	MOTA	98	CB	LYS A	83		41.096	5.625	-11.687	1.00 22.02	A
10	MOTA	99	CG ·	LYS A	83		40.062	6.326	-12.550	1.00 28.93	A
	MOTA	100	CD	LYS A	83		38.974	5.355	-12.981	1.00 34.20	A
	MOTA	101	CE	LYS A	83		37.909	6.042	-13.824	1.00 38.10	A
	MOTA	102	NZ	LYS A	83		37.179	7.086	-13.043	1.00 43.33	A
	MOTA	103	С	LYS A	83		41.913	7.702	-10.541	1.00 20.74	A
15	ATOM	104	0	LYS A	83		41.084	7.606	-9.635	1.00 20.98	A
	MOTA	105	N	PHE A	84		42.513	8.848	-10.835	1.00 19.99	A
	ATOM	106	CA	PHE A	84		42.188	10.049	-10.083	1.00 18.63	A
	MOTA	107	CB	PHE A	84		43.279		-10.258	1.00 18.95	A
	ATOM	108	CG	PHE A	84		44.571	10.741	-9.587	1.00 17.68	A
20	ATOM	109		PHE A	84		45.498		-10.224	1.00 18.16	А
	MOTA	110		PHE A	84		44.843	11.183	-8.299	1.00 19.66	A
	MOTA	111		PHE A	84		46.676	9.556	-9.589	1.00 18.09	A
•	ATOM	112		PHE A	84		46.021	10.816	-7.653	1.00 18.89	A
	MOTA	113	cz	PHE A	84		46.936	10.002	-8.301	1.00 17.33	A
25	ATOM	114	C ·	PHE A	84		40.834	10.617	-10.460	1.00 19.69	A
	ATOM	115	0	PHE A	84		40.391	10.489		1.00 20.72	A
	ATOM	116	N	GLY A	85		40.178	11.233	-9.484	1.00 16.80	. A
	MOTA	117	CA	GLY A	85		38.872	11.810	-9.716	1.00 17.73	A
	MOTA	118	С	GLY A	85		38.819	13.280	-9.346	1.00 18.75	A
30	ATOM	119	0	GLY A	. 85		39.740	14.043	-9.650	1.00 18.45	A
	ATOM	120	N	LYS A	86		37.753	13.673	-8.659	1.00 16.00	A
	ATOM	121	CA	LYS A	86		37.571	15.064	-8.278	1.00 18.26	A
	MOTA	122	СВ	LYS A	86		36.133	15.302	-7.812	1.00 19.00	A
0.5	ATOM	123	CG	LYS A	86		35.793	14.660	-6.481	1.00 21.55	A
35	ATOM	124	CD	LYS A	86		34.368	14.981	-6.066	1.00 26.48 1.00 31.92	A A
	ATOM	125	CE	LYS A	86		33.994 32.568	14.239	-4.793 -4.412	1.00 31.92	A
	MOTA	126	NZ	LYS A	86		38.523	14.457 15.571	-7.202	1.00 33.30	A
	MOTA	127	C	LYS A	86 86		39.045	14.807	-6.385	1.00 16.37	Ā
40	ATOM	128 129	0	ILE A	87		38.737	16.881	-7.227	1.00 10.77	A
40	ATOM	130	N CA	ILE A	87		39.577	17.554	-6.256	1.00 17.00	A
	ATOM ATOM	131	CB	ILE A	87		39.994	18.952	-6.772	1.00 19.60	A
	ATOM	132.	CG2	ILE A	87		40.593	19.786	-5.628	1.00 18.73	A
	ATOM	133		ILE A	87		40.968	18.786	-7.945	1.00 21.16	A
45	ATOM	134		ILE A	87		41.412	20.087	-8.588	1.00 25.26	A
73	ATOM	135	CDI	ILE A	87		38.731	17.709	-4.997	1.00 19.67	A
	ATOM	136	Ö	ILE A	87		37.628	18.249	-5.052	1.00 20.41	A
	ATOM	137	N	LEU A	88		39.240	17.229	-3.867	1.00 19.15	A
	ATOM	138	CA	LEU A	88		38.508	17.324	-2.611	1.00 20.68	A
50	ATOM	139	CB	LEU A	88		38.870	16.151	-1.700	1.00 19.97	A
30	ATOM	140	CG	LEU A	88		38.529	14.759	-2.237	1.00 19.24	A
	ATOM	141		LEU A	88		39.090	13.692	-1.311	1.00 21.41	A
	ATOM	142		LEU A	88	•	37.029	14.622	-2.359	1.00 18.84	A
	ATOM	143	C	LEU A	88		38.815	18.632	-1.901	1.00 23.11	A
55	ATOM	144	Ö	LEU A	88		37.999	19.146	-1.139	1.00 25.10	A
	ATOM	145	N	GLY A	89		39.997	19.174	-2.149	1.00 24.09	A
	ATOM	146	CA	GLY A	89		40.367	20.418	-1.507	1.00 24.27	A
	ATOM	147	С	GLY A	89		41.658	20.954	-2.078	1.00 25.47	A
	ATOM	148	0 -		89		42.445		-2.666	1.00 22.19	A

	•		•							
	ATOM	149	N	GLU .	A 90	41.870	22.254	-1.906	1.00 26.22	A
	MOTA	150	CA	GLU .	A 90	43.064	22.924	-2.404	1.00 29.96	. A
	MOTA	151	CB	GLU .	A 90	42.698	23.814	-3.596	1.00 30.75	A
	ATOM	152	CG	GLU .	A 90	42.267	23.038	-4.831	1.00 34.32	A
5	ATOM	153		GLU			23.930	-5.927	1.00 34.32	A
•	ATOM	154		GLU				-5.764		
				GLU			24.456		1.00 40.57	A
	ATOM	155					24.110	-6.952	1.00 40.90	Α
	MOTA	156	С	GLU Z			23.768	-1.313	1.00 30.68	A
	ATOM	157	0	GLU			24.574	-0.668	1.00 32.83	A
10	ATOM	158	N	GLY I		45.006	23.566	-1.104	1.00 29.66	A
	ATOM	159	CA	GLY I	A 91	45.724	24.332	-0.104	1.00 29.40	A
	ATOM	160	С	GLY I	A 91	46.795	25.151	-0.798	1.00 29.98	A
	ATOM	161	0	GLY 2	A 91	46.894	25.130	-2.028	1.00 28.16	A
	ATOM	162	N	SER I			25.870	-0.029	1.00 28.30	A
15	ATOM	163	CA	SER Z			26.681	-0.633	1.00 30.50	A
	ATOM	164	CB	SER A			27.717	0.370	1.00 30.30	
	ATOM	165	OG	SER A						A
							27.099	1.593	1.00 40.94	A
	MOTA	166	С	SER A			25.843	-1.164	1.00 29.77	A
	ATOM	167	0	SER A			26.221	-2.143	1.00 30.46	A
20	MOTA	168	N	PHE A			24.703	-0.536	1.00 27.65	A
	ATOM	169	CA	PHE A			23.855	-0.995	1.00 26.34	A
	ATOM	170	CB	PHE A	A 93	52.281	23.785	0.068	1.00 27.95	A
	ATOM	171	CG	PHE A	A 93	52.861	25.117	0.406	1.00 31.06	A
	ATOM	172	CD1	PHE A	A 93	52.283	25.909	1.392	1.00 29.96	A
25	ATOM	173	CD2	PHE A	A 93	53.949	25.613	-0.308	1.00 31.38	A
	ATOM	174		PHE A		52.779	27.181	1.665	1.00 32.69	A
	ATOM	175		PHE A			26.883	-0.044	1.00 32.63	A
	ATOM	176		PHE A		53.864	27.670	0.945	1.00 32.03	A
				PHE A			22.445			
20	ATOM	177	C			50.759		-1.365	1.00 25.39	A
30	ATOM	178	0	PHE A		51.601	21.559	-1.522	1.00 24.59	A
	MOTA	179	N	SER A		49.457	22.235	-1.519	1.00 23.63	A
	ATOM	180	CA	SER A		48.965	20.912	-1.860	1.00 21.43	A
	MOTA	181	CB	SER A		49.017	20.013	-0.628	1.00 21.42	A
	MOTA	182	OG	SER A	94	48.091	20.475	0.340	1.00 21.19	A
35	MOTA	183	С	SER A	94	47.539	20.925	-2.378	1.00 19.82	A
	ATOM	184	0	SER A	94	46.795	21.882	-2.173	1.00 18.76	A
	ATOM	185	N	THR A	A 95	47.174	19.832	-3.038	1.00 19.38	A
	MOTA	186	CA	THR A	A 95	45.840	19.637	-3.580	1.00 17.98	A
	MOTA	187	СВ	THR A		45.818	19.818	-5.110	1.00 19.25	A
40	ATOM	188		THR A		46.196	21.162	-5.434	1.00 22.04	A
. •	ATOM	189		THR A		44.421	19.549	-5.661	1.00 17.61	A
	ATOM	190	C	THR A		45.455	18.201	-3.243	1.00 17.01	A
	ATOM	191	õ.	THR A		46.212	17.264	-3.524	1.00 17.10	A
		192	,							
45	ATOM		N	VAL A		44.295	18.024	-2.623	1.00 16.53	A
45	ATOM	193	CA	VAL A		43.845	16.685	-2.266	1.00 16.05	A
	ATOM	194	CB	VAL A		43.170	16.672	-0.886	1.00 16.32	A
	ATOM	195		VAL A		42.741	15.249	-0.532	1.00 18.02	A
	ATOM	196		VAL A		44.145	17.206	0.168	1.00 16.69	A
	ATOM	197	С	VAL A	96	42.875	16.207	-3.335	1.00 16.42	A
50	ATOM	198	0	VAL A	96	41.906	16.892	-3.665	1.00 16.47	A
	ATOM	199	N	VAL A	97	43.157	15.033	-3.888	1.00 16.80	A
	ATOM	200	CA	VAL A		42.338	14.471	-4.949	1.00 16.72	A
	ATOM	201	CB	VAL A		43.153	14.354	-6.255	1.00 18.43	A
	ATOM	202		VAL A		42.249	13.927	-7.404	1.00 10.43	A
55	MOTA	202		VAL A		43.831	15.685	-6.569	1.00 17.84	
JJ										A
	ATOM	204	C	VAL A		41.812	13.091	-4.583	1.00 16.77	A
	MOTA	205	0	VAL A		42.532	12.270	-4.014	1.00 17.13	A
	ATOM	206	N	LEU A		40.545	12.845	-4.895	1.00 16.62	A
	ATOM	207	CA	LEU A	98	39.947	11.548	-4.624	1.00 17.04	A

	ATOM	208	СВ		98	38.424	11.633		1.00 16.89	А
	MOTA	209			98	37.635	10.342			A
	ATOM	210		1 LEU A	98	37.990	9.762	-3.146	1.00 20.07	А
_	ATOM	211		2 LEU A	98	36.143	10.627		1.00 17.93	A
5	ATOM	212	С	LEU A	98	40.512	10.597	,	1.00 17.38	A
	ATOM	213	0	LEU A	98	40.527	10.920		1.00 18.60	A
	ATOM	214	N	ALA A	99	40.995	9.438		1.00 17.13	A
	ATOM	215	CA		99	41.570	8.466		1.00 18.42	A
10	ATOM	216	CB	ALA A	99	43.090	8.524		1.00 14.76	. A
10	ATOM	217	C	ALA A	99	41.102	7.055		1.00 21.40	A
	MOTA	218	0	ALA A	99	40.941	6.691		1.00 22.52	A
	ATOM	219	N	ARG A 1		40.878	6.261		1.00 19.77	A
	ATOM ATOM	220	CA	ARG A 1		40.459	4.884	-6.693	1.00 20.85	A
15	ATOM	221 222	CB	ARG A 1		39.202	4.585	-7.518	1.00 24.22	A
13	ATOM	223	CG	ARG A 1		38.608	3.205	-7.256	1.00 31.78	A
	ATOM	224	CD NE	ARG A 1 ARG A 1		37.326	2.979	_	1.00 36.24	A
	ATOM	225	CZ	ARG A 1		36.213	3.818	-7.594	1.00 41.40	A
	ATOM	226		L ARG A 1		35.566	3.662	-6.439	1.00 42.05	
20	ATOM	227		ARG A 1		35.912 34.559	2.696	-5.598	1.00 40.67	A
20	ATOM	228	C	ARG A 1		41.613	4.468 3.985	-6.128 -7.129	1.00 43.65	A
	ATOM	229	ŏ	ARG A 1		42.078	4.065	-8.271	1.00 18.63 1.00 19.49	A
	ATOM	230	N	GLU A 1		42.102	3.157	-6.212	1.00 19.49	A A
	ATOM	231	CA	GLU A 1		43.196	2.246	-6.533	1.00 16.43	A
25	ATOM	232	СВ	GLU A 1		43.774	1.637	-5.248	1.00 16.79	A
	ATOM	233	CG	GLU A 1		44.917	0.657	-5.488	1.00 16.73	A
	MOTA	234	CD	GLU A 1		45.501	0.115	-4.200	1.00 18.20	A
	ATOM	235	OEI	GLU A 1		44.733	-0.081	-3.239	1.00 18.32	A
	ATOM	236	OE2	GLU A 1	01	46.725	-0.132	-4.150	1.00 17.14	A
30	ATOM`	237	С	GLU A 1	01	42.625	1.152	-7.442	1.00 17.92	A
	ATOM	238	0	GLU A 1	01	41.681	0.462	-7.069	1.00 18.02	A
	ATOM	239	Ν.	LEU A 1	02	43.198	1.002	-8.632	1.00 19.06	A
	ATOM	240	CA	LEU A 1	02 -	42,718	0.025	-9.607	1.00 20.71	· A
	ATOM .	241	CB	LEU A 1		43.569	0.097	-10.878	1.00 23.42	A
35	ATOM	242	CG	LEU A 1		43.531		-11.642	1.00 25.30	A
	ATOM	243		LEU A 1		44.577		-12.748	1.00 27.88	A
	ATOM	244		LEU A 1		42.140		-12.214	1.00 26.79	A
	ATOM	245	C	LEU A 1		42.671	-1.418	-9.125	1.00 21.62	Α
40	ATOM	246	0	LEU A 10		41.668	-2.103	-9.305	1.00 21.09	A
40	ATOM	247	N	ALA A 1		43.753	-1.874	-8.507	1.00 19.38	A
	ATOM ATOM	248 249	CA	ALA A 10		43.836	-3.249	-8.035	1.00 20.87	A
	ATOM	250	СВ	ALA A 10 ALA A 10		45.284 42.919	-3.571	-7.671	1.00 19.23	A
•	ATOM	251	0	ALA A 10		42.703	-3.629	-6.872	1.00 19.92	A
45	ATOM	252	N	THR A 10		42.703	-4.815 -2.643	-6.628	1.00 20.38	A
7.5	ATOM	253	CA	THR A 10		41.517	-2.927	-6.175 -5.018	1.00 18.12 1.00 17.15	A
	ATOM	254	CB	THR A 10		42.212	-2.327	-3.717	1.00 17.15	A A
	ATOM	255		THR A 10		42.456	-1.070	-3.773	1.00 19.34	A
	ATOM	256		THR A 10		43.536	-3.219	-3.529	1.00 13.20	A
50	ATOM	257	C	THR A 10		40.159	-2.247	-5.026	1.00 17.02	Ā
	ATOM	258	Ō.	THR A 10		39.259	-2.648	-4.285	1.00 18.70	A
	ATOM	259	N	SER A 10		40.034	-1.207	-5.847	1.00 19.65	A
	ATOM	260	CA	SER A 10		38.819	-0.400	-5.967	1.00 19.37	A
	ATOM	261	СВ	SER A 10		37.598	-1.304	-6.173	1.00 21.81	A
55	ATOM	262	OG	SER A 10		36.431	-0.539	-6.412	1.00 23.01	A
	ATOM	263	С	SER A 10	5	38.644	0.447	-4.701	1.00 18.99	A
	ATOM	264	0	SER A 10		37.602	1.070	-4.488	1.00 18.66	Α
	ATOM	265	N	ARG A 10		39.674	0.468	-3.861	1.00 16.84	A
	ATOM	266	CA	ARG A 10	6 .	39.655	1.267	-2.634	1.00 16.21	Α

	ATOM	267	CB	ARG	A	106		40.827	0.886	-1.723	1.00 16.41	A
	ATOM	268	CG	ARG	Α	106		40.619	-0.367	-0.906	1.00 15.49	A
	ATOM	269	CD	ARG	Α	106		41.887	-0.755	-0.170	1.00 17.43	Α
	ATOM	270	NE	ARG	Α	106		41.620	-1.792	0.824	1.00 20.47	A
5 '	ATOM	271	CZ	ARG	A	106		42.548	-2.568	1.371	1.00 20.24	A
	ATOM	272	NH1	ARG	Α	106		43.821	-2.433	1.017	1.00 17.80	A
	ATOM	273	NH2	ARG	Α	106		42.198	-3.468	2.285	1.00 20.14	A
	ATOM	274	С	ARG	Α	106		39.785	2.746	-2.981	1.00 17.37	A
	ATOM	275	0	ARG				40.514	3.103	-3.902	1.00 17.75	A
10	ATOM	276	N	GLU				39.085	3.599	-2.240	1.00 16.06	A
	ATOM	277	CA	GLU				39.156	5.039	-2.461	1.00 20.80	A
	ATOM	278	СВ	GLU				37.779	5.694	-2.337	1.00 22.93	A
•	ATOM	279	CG	GLU				36.711	5.171	-3.269	1.00 30.87	A
	ATOM	280	CD	GLU				35.431	5.975	-3.148	1.00 32.40	A
15	ATOM	281	OE1					35.262	6.939	-3.923	1.00 32.40	A
15	ATOM	282		GLU				34.608	5.654	-2.263	1.00 35.74	A
	ATOM	283	C	GLU				40.053	5.678	-1.410	1.00 30.00	A
	ATOM	284	Ö	GLU			•	39.891	5.427	-0.220	1.00 10.33	A
	ATOM	285	N	TYR				40.988	6.507	-1.852	1.00 19.21	A
20	ATOM	286	CA	TYR				41.883	7.209	-0.942	1.00 15.70	· A
20	ATOM	287	CB	TYR				43.325	6.728	-1.104	1.00 15.30	A
	ATOM	288	CG	TYR				43.523	5.328	-0.612	1.00 15.30	A
											1.00 16.35	A
	ATOM	289	CD1					43.765	5.066 3.769	0.746 1.201	1.00 18.48	. A
25	ATOM	290	CE1	TYR				44.046		-1.511	1.00 18.46	
25	ATOM	291	CD2					43.701	4.268			A
	ATOM	292	CE2					43.980	2.981	-1.075	1.00 17.28 1.00 19.17	A
	ATOM	293	CZ	TYR				44.152	2.736	0.276		A
	. ATOM	294	ОН	TYR			_	44.440	1.461	0.688	1.00 19.38	A
	ATOM	295	С	TYR			-	41.850	8.687	-1.292	1.00 16.80	A
30	MOTA	296	0	TYR				41.560	9.058	-2.431	1.00 15.22	A
	ATOM	297	N	ALA				42.132	9.528	-0.306	1.00 14.61	A
	ATOM	298	CA	ALA				42.207	10.957	-0.539	1.00 14.30	A
	MOTA	299	СВ	ALA			•	41.671	11.726	0.661	1.00 14.78	A
	ATOM	300	С	ALA				43.713	11.136	-0.667	1.00 16.79	· A
35	ATOM	301	0	ALA				44.450	10.983	0.317	1.00 16.52	A
	MOTA	302	N	ILE				44.182	11.410	-1.881	1.00 14.80	A.
	MOTA	303	CA	ILE				45.609	11.574	-2.093	1.00 15.80	A
	MOTA	304	СВ	ILE				46.065	10.863	-3.396	1.00 16.85	A
	ATOM	305	CG2					47.550	11.098	-3.632	1.00 16.80	A
40	ATOM	306	CG1	ILE				45.774	9.358	-3.284	1.00 17.76	A
	ATOM	307		ILE				46.308	8.513	-4.437	1.00 16.07	A
	ATOM	308	С	ILE				46.004	13.045	-2.129	1.00 17.78	A
	ATOM	309	0	ILE				45.534	13.813	-2.976	1.00 16.24	A
	ATOM	310	N	LYS				46.846	13.435	-1.177	1.00 16.15	A
45	ATOM	311	CA	LYS				47.326	14.808	-1.100	1.00 17.20	A
	ATOM	312	CB	LYS				47.700	15.176	0.344	1.00 17.41	Α
	ATOM	313	CG	LYS				48.350	16.547	0.464	1.00 20.71	A
	ATOM	314	CD	LYS				48.585	16.971	1.910	1.00 24.25	A
	ATOM	315	CE	LYS				47.288	17.381	2.598	1.00 29.46	A
50	ATOM	316	NZ	LYS				47.516	17.866	4.000	1.00 30.50	A
	ATOM	317	С	LYS				48.551	14.890	-1.994	1.00 16.41	A
	ATOM	318	0	LYS				49.509	14.137	-1.813	1.00 18.20	A.
	ATOM	319	N	ILE				48.509	15.798	-2.963	1.00 15.87	A
	ATOM	320	CA	ILE				49.606	15.967	-3.907	1.00 17.28	A
55	MOTA	321	CB	ILE				49.079	15.911	-5.358	1.00 16.43	A
	ATOM	322		ILE				50.235	15.998	-6.341	1.00 15.12	A
	ATOM	323		ILE				48.293	14.609	-5.565	1.00 16.82	Α
	ATOM	324	CD1	ILE				47.580	14.511	-6.904	1.00 18.47	A
	MOTA	325	С	ILE	A	112		50.307	17.301	-3.663	1.00 19.03	A

	. ATOM	326	0	ILE A 1	112	49.669	.18.350	-3.635	1.00	19.15	A
	ATOM	327	N	LEU A 1	113	51.622	17.245	-3.472		20.22	. A
	ATOM	328	CA	LEU A J		52.416	18.442	-3.214		22.36	. A
	ATOM	329	СВ	LEU A 1		52.995	18.397	-1.794		22.13	. A
5	ATOM	330	CG	LEU A 1	113	52.042	18.063	-0.646		22.46	. A
	ATOM	331	CDI	LEU A 1	113	51.866	16.557	-0.553		23.81	A
	ATOM	332		LEU A 1		52.603	18.595	0.660		23.68	A
	ATOM	333	С	LEU A 1		53.560	18.547	-4.215		23.37	A
	ATOM	334	0	LEU A 1		54.300	17.586	-4.424		23.11	A
10	ATOM	335	N	GLU A 1	14	53.706	19.714	-4.834		23.88	A
	ATOM	336	CA	GLU A 1		54.771	19.920	-5.806		26.00	A
	ATOM	337	CB	GLU A 1	14	54.435	21.111	-6.706		27.74	A
	ATOM	338	CG	GLU A 1	.14	55.533	21.452	-7.696		35.07	A
	ATOM	339	CD	GLU A 1	.14	55.220	22.696	-8.497		39.24	A
15	ATOM	340	OE1	GLU A 1	14	54.808	23.703	-7.885		41.45	A
	ATOM	341		GLU A 1		55.395	22.670	-9.736		44.05	A
	ATOM	342	С	GLU A 1		56.087	20.163	-5.067		24.37	A
	ATOM	343	0	GLU A 1		56.186	21.071	-4.238		24.43	A
	ATOM	344	N	LYS A 1		57.096	19.350	-5.360		24.10	A
20	ATOM	345	CA	LYS A 1	15	58.376	19.493	-4.678		24.93	A
	MOTA	346	CB	LYS A 1	15	59.339	18.373	-5.103		23.72	A
	ATOM	347	CG	LYS A 1		59.139	17.080	-4.308		23.09	A
	ATOM	348	CD	LYS A 1	15	60.064	15.944	-4.743		21.92	A
	ATOM	349	CE	LYS A 1	15	59.691	15.400	-6.117		22.42	A
25	ATOM	350	NZ	LYS A 1	15	60.447	14.150	-6.448		19.71	A
	ATOM	351	С	LYS A 1	15	59.031	20.858	-4.868		26.87	A
	ATOM	352	0	LYS A 1	15	59.492	21.469	-3.903		26.17	A
	ATOM	353	N	ARG A 1	16	59.058	21.348	-6.102		28.73	A
	ATOM	354	CA	ARG A 1	16	59.678	22.638	-6.380		29.66	A
30	ATOM	355	CB	ARG A 1	16	59.533	22.980	-7.868		31.29	Α
	ATOM	356	CG	ARG A 1	16	60.047	24.361	-8.267		33.19	A
	ATOM	357	CD	ARG A 1	16	61.368	24.710	-7.590	1.00	35.13	Α
	ATOM	358	NE	ARG A 1	16	62.329	23.612	-7.618	1.00	36.42	A
	ATOM	[:] 359	CZ	ARG A 1	16	63.510	23.648	-7.009	1.00	36.18	A
35	ATOM	360	NH1	ARG A 1	16	63.871	24.729	-6.332	1.00	36.12	A
	ATOM	361	NH2	ARG.A 1	16	64.324	22.602	-7.067	1.00	35.77	A
	ATOM	362	С	ARG A 1	16	59.097	23.761	-5.519	1.00	29.70	A
	MOTA	363	0	ARG A 1	16	59.843	24.515	-4.889	1.00	29.16	A
	ATOM	364	N	HIS A 1		57.773	23.862	-5.472	1.00	27.22	A
40	MOTA	365	CA	HIS A 1	17	57.126	24.903	-4.681	1.00	26.33	À
	MOTA	_. 366	CB	HIS A 1		55.606	24.835	-4.848	1.00	28.41	A
	MOTA	367	CG	HIS A 1		54.881	26.005	-4.258	1.00	31.82	A
	MOTA	368		HIS A 1		55.309	27.249	-3.935	1.00	33.19	A
	MOTA	369		HIS A 1		53.536	25.974	-3.961	1.00	34.30	A
45	MOTA	370		HIS A 1		53.165	27.148	-3.480	1.00	34.58	A
	ATOM	371		HIS A 1		54.222	27.940	-3.455	1.00	35.18	Α
	ATOM	372	С	HIS A 1		57.477	24.780	-3.202		26.22	Α
	ATOM	373	0	HIS A 1		57.737	25.776	-2.534	1.00	25.67	A
	ATOM	374	N	ILE A 11		57.469	23.554	-2.689		24.94	A
50	ATOM	375	CA	ILE A 11		57.792	23.315	-1.285	1.00	23.94	A
	MOTA	376	CB	ILE A 11		57.711	21.812	-0.952	1.00	23.50	A
	ATOM	377		ILE A 11		58.374	21.533	0.389	1.00	23:76	A
	ATOM	378		ILE A 11		56.246	21.362	-0.959		24.42	A
~~	ATOM	379		ILE A 11		56.066	19.858	-0.834		28.06	A
55	ATOM	380	С	ILE A 11		59.195	23.821	-0.958		23.78	A
	MOTA	381	0	ILE A 11		59.402	24.495	0.048		23.49	A
	ATOM	382	N	ILE A 11		60.153	23.489	-1.815	1.00	23.46	A
	ATOM	383	CA	ILE A 11		61.534	23.913	-1.619		25.13	À
	MOTA	384	CB	ILE A 11	١9	62.467	23.250	-2.664	1.00	24.25	A

								•			•
-	ATOM	385		2 ILE A			63.858	23.890	-2.617	1.00 22.4	7 A
	ATOM	386		1 ILE A			62.540	21.738	-2.395		
	ATOM	387		1 ILE A			63.327	20.945	-3.439	1.00 24.6	
_	MOTA	388		ILE A			61.667		-1.705	1.00 25.9	
5	ATOM	389		ILE A			62.330	26.051	-0.872		
	MOTA	390		LYS F			61.028		-2.704	1.00 27.6	
	ATOM	391					61.100		-2.879	1.00 30.2	
	MOTA	392					60.242	27.940	-4.060	1.00 32.3	
••	ATOM	393					60.674	27.407	-5.409	1.00 39.3	
10	ATOM	394					59.765		-6.512	1.00 45.1	
	ATOM	395		LYS A			58.294		-6.218	1.00 46.4	
	ATOM	396		LYS A			57.363		-7.252	1.00 46.4	9 A
	ATOM	397		LYS A			60.647		-1.638	1.00 30.8	9 · A
1.5	ATOM	398		LYS A			51.303		-1.217	1.00 32.4	
15	ATOM	399		GLU A		Į.	59.527	27.825	-1.055	1.00 29.83	2 A
	ATOM	400		GLU A			58.986	28.488	0.128	1.00 30.33	
	ATOM	401		GLU A			7.455	28.416	0.117	1.00 33.04	4 A
	ATOM	402		GLU A		į	6.794	29.021	-1.120	1.00 36.49	5 A
	MOTA	403		GLU A			7.221	30.456	-1.373	1.00 39.88	
20	ATOM	404		l GLU A		į	7.200	31.264	-0.420	1.00 40.53	
	MOTA	405					7.573	30.778	-2.529	1.00 43.24	A
	MOTA	406		GLU A			9.511	27.930	1.451	1.00 30.37	
	ATOM	407	0	GLU A			8.946	28.204	2.513	1.00 31.24	
0.5	ATOM .	408	N	ASN A			0.588	27.151	1.390	1.00 29.03	3 A
25	ATOM	409	CA	ASN A			1.183	26.573	2.594	1.00 28.46	5 A
	MOTA	410	CB	ASN A			1.836	27.673	3.436	1.00 31.28	A
	ATOM	411	CG	ASN A			2.945	28.395	2.698	1.00 34.12	A
	MOTA	412		. ASN A			2.697	29.143	1.754	1.00 35.57	Α.
0.0	ATOM	413		ASN A			4.181	28.169	3.127	1.00 35.73	A
30	ATOM	414	С	ASN A		6	0.157	25.835	3.456	1.00 26.89	A
	ATOM	415	0	ASN A			0.085	26.055	4.663	1.00 27.23	A
	MOTA	416	N	LYS A			9.375	24.955	2.842	1.00 23.99	A
	ATOM	417	CA	LYS A			8.358	24.210	3.574	1.00 22.43	A
25	ATOM	418	СВ	LYS A			7.031	24.248	2.810	1.00 21.97	A
35	ATOM	419	CG	LYS A			6.475	25.645	2.599	1.00 25.68	A
	ATOM	420	CD	LYS A			6.253	26.354	3.927	1.00 27.54	
	MOTA	421	CE	LYS A			5.822	27.796	3.716	1.00 31.30	A
	ATOM	422	NZ	LYS A			5.756	28.540	5.004	1.00 33.21	
40	MOTA	423	С	LYS A			8.748	22.759	3.821	1.00 22.20	
40	ATOM	424	0	LYS A			7.924	21.960	4.264	1.00 22.50	
	ATOM	425	И	VAL A			9.997	22.412	3.535	1.00 20.59	
	ATOM ATOM	426	CA	VAL A			0.439	21.039	3.730	1.00 20.25	
		427	CB	VAL A			1.922	20.850	3.328	1.00 19.43	
45	ATOM	428		VAL A		_	2.346	19.407	3.573	1.00 18.69	A
73	MOTA	429		VAL A			2.104	21.195	1.853	1.00 18.21	A
	ATOM	430	C	VAL A			0.236	20.561	5.163	1.00 19.53	A
	ATOM	431	0	VAL A			9.841	19.418	5.385	1.00 20.02	A
	ATOM ATOM	432	И	PRO A			0.513	21.422	6.159	1.00 20.01	A
50	ATOM	433 434	CD	PRO A			1.178	22.738	6.118	1.00 18.69	A
50			CA	PRO A			318	20.979	7.544	1.00 19.88	A
	ATOM	435	CB	PRO A			7.793	22.180	8.363	1.00 19.95	A
	ATOM	436	CG	PRO A			1.839	22.805	7.479	1.00 18.85	A
	ATOM	437	С	PRO A			3.848	20.642	7.824	1.00 19.76	A
55	ATOM	438	0	PRO A			3.544	19.700	8.550	1.00 16.99	A
"	ATOM	439	N	TYR A			.947	21.418	7.235	1.00 18.98	A
	ATOM	440	CA	TYR A			5.516	21.220	7.435	1.00 21.97	A
	ATOM	441	CB	TYR A			.752	22.448	6.933	1.00 25.17	A
	ATOM	442	CG CD1	TYR A			.040	23.690	7.748	1.00 30.98	A
	ATOM	443	CD1	TYR A	T 2 P	55	.438	23.886	8.991	1.00 33.95	· A

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	ATOM	444	CE	LTYF	A S	126	55.721	25.015	9.763	1.00 36.60	
	ATOM	445				126	56.938	24.657	7.292	1.00 35.43	· A
	ATOM	446	CE2	? TYF	R A	126	57.231	25.792	8.058	1.00 37.20	· : • · A
	ATOM	447	CZ			126	56.618	25.962	9.291	1.00 37.40	A
5	ATOM	448	OH			126	56.903	27.073	10.052	1.00 40.85	A
	MOTA	449	С			126	55.990	19.956	6.762	1.00 21.35	A
	ATOM	450	0	TYP	A	126	55.265	19.175	7.383	1.00 20.49	A
	ATOM	451	N	IAV	A	127	56.354	19.746	5.501	1.00 18.16	A
	ATOM	452	CA			127	55.892	18.562	4.790	1.00 17.58	A
10	ATOM	453	CB			127	56.308	18.596	3.308	1.00 17.45	A
	MOTA	454		. VAL			55.786	17.350	2.600	1.00 17.97	Α
	ATOM	455	CG2	VAL			55.751	19.850	2.641	1.00 14.90	A
	. ATOM	456	С			127	56.459	17.306	5.448	1.00 18.39	A
	MOTA	457	0			127	55.769	16.298	5.583	1.00 18.14	A
15	MOTA	458	N	THR	A	128	57.716	17.381	5.869	1.00 17.50	A
	MOTA	459	CA			128	58.375	16.260	6.530	1.00 18.54	A
	ATOM	460	CB			128	59.861	16.586	6.805	1.00 18.01	A
	ATOM	461		THR			60.537	16.804	5.559	1.00 21.14	A
	ATOM	462	CG2				60.536	15.446	7.545	1.00 17.95	Α
20	ATOM	463	С			128	57.676	15.941	7.856	1.00 19.49	A
	MOTA	464	0			128	57.438	14.776	8.179	1.00 18.76	A
	MOTA	465	N			129	57.345	16.981	8.619	1.00 19.60	A
	ATOM	466	CA			129	56.673	16.804	9.904	1.00 20.12	A
	ATOM	467	CB			129	56.534	18.144	10.621	1.00 21.33	A
25	ATOM	468	CG			129	55.948	18.029	12.023	1.00 28.02	A
	ATOM	469	CD			129	55.721	19.404	12.597	1.00 31.25	Α
	MOTA	470	NE			129	56.940	20.205	12.560	1.00 37.78	A
	ATOM	471	CZ			129	56.962	21.524	12.391	1.00 40.10	A
20	ATOM	472		ARG			55.828	22.197	12.239	1.00 40.03	A
30	ATOM	473				129	58.119	22.170	12.374	1.00 44.58	A
	ATOM	474	C			129	55.288	16.186	9.729	1.00 20.08	A
	ATOM ATOM	475 476	И О			129 130	54.891 54.553	15.305	10.496	1.00 20.40	A
	ATOM	477	CA			130	53.222	16.654	8.724 8.454	1.00 18.79 1.00 20.10	A
35	ATOM	478	CB			130	52.638	16.125 16.749	7.183	1.00 20.10	A A
55	ATOM	479	CG			130	51.350	16.087	6.708	1.00 13.32	A
	ATOM	480	CD			130	50.581	16.933	5.707	1.00 27.03	A
	ATOM	481	OE1				51.216	17.528	4.814	1.00 23.72	A
	ATOM	482		GLU			49.339	16.996	5.807	1.00 30.74	A
40	ATOM	483	C			130	53.301	14.615	8.295	1.00 30.71	A
. •	ATOM	484	ō			130	52.553	13.875	8.935	1.00 18.37	A
	ATOM	485	N	ARG			54.219	14.162	7.447	1.00 20.41	A
	ATOM	486	CA	ARG			54.397	12.735	7.202	1.00 22.45	A
	ATOM	487	CB	ARG	Α	131	55.442	12.511	6.098	1.00 25.16	A
45	ATOM	488	CG	ARG	Α	131	55.742	11.043	5.840	1.00 28.75	A
	ATOM	489	CD	ARG			56.736	10.837	4.708	1.00 33.75	A
	ATOM	490	NE	ARG			57.020	9.415	4.520	1.00 40.07	A
	ATOM	491	CZ	ARG	Α	131	57.756	8.915	3.532	1.00 43.07	A
	ATOM	492	NH1	ARG	Α	131	58.293	9.721	2.625	1.00 44.91	Α
50	ATOM	493	NH2	ARG	Α	131	57.955 ·	7.606	3.449	1.00 44.45	A
	MOTA	494	С	ARG	Α	131	54.820	11.982	8.466	1.00 23.24	A
	ATOM	495	0	ARG	А	131	54.241	10.948	8.804	1.00 23.86	A
	ATOM	496	N	ASP	Α	132	55.831	12.497	9.160	1.00 21.99	Α
	ATOM .	497	CA	ASP			56.318	11.850.	10.370	1.00 22.04	A
55	ATOM	498	CB	ASP			57.570	12.564	10.888	1.00 23.72	. А
	MOTA		· CG	ASP			58.750	12.442	9.932	1.00 27.77	A
	MOTA	500		ASP			58.681	11.620	8.989	1.00 27.34	A
	MOTA	501	OD2	ASP			59.753	13.163	10.128	1.00 28.70	A
	ATOM	502	С	ASP	A	132	55.258	11.772	11.474	1.00 21.69.	A

	ATOM	503	0	ASP	Α	132	55.077	10.723	12.092	1.00	22.75		Α
	ATOM	504	N	VAL	Α	133	54.551	12.868	11.725		19.54		A
	ATOM	505	CA	VAL	Α	133	53.525	12.843	12.759		18.52		A
	ATOM	506	CB			133	52.908	14.244	12.990		19.26		A
5	ATOM	507		VAL			51.708	14.135	13.918		18.79		A
_	ATOM	508		VAL			53.953	15.180	13.604		18.80		A
	ATOM	509	C			133	52.419	11.854	12.398		19.46		A
	ATOM	510	o			133	52.419	10.991	13.200		19.94		A
	ATOM	511	N	MET				11.957					
10							51.878		11.187		19.15		A
10	ATOM	512	CA	MET			50.807	11.052	10.792		21.25		A
	ATOM	513	CB	MET			50.309	11.381	9.383		17.34		A
	ATOM	514	CG	MET			49.615	12.730	9.302		20.00		A
	ATOM	515	SD			134"	48.643	12.952	7.798		24.21		A
٠	ATOM	516	CE	MET			47.033	12.434	8.400		23.20		A
15	ATOM	517	С	MET			51.203	9.582	10.881		22.43		Α
	ATOM	518	0	MET	Α	134	50.384	8.741	11.249		23.82		Α
	ATOM	519	N	SER	Α	135	52.454	9.273	10.556	1.00	23.09		Α
	ATOM	520	CA	SER	Α	135	52.939	7.895	10.615	1.00	26.13		Α
	ATOM	521	CB	SER	Α	135	54.356	7.798	10.039	1.00	26.17		Α
20	ATOM	522	OG	SER	Α	135	54.383	8.177	8.673	1.00	31.91		Α
	ATOM	523	C	SER	Α	135	52.957	7.358	12.045	1.00	26.58		Α
	ATOM	524	0	SER	A	135	52.926	6.148	12.261	1.00	26.42		Α
	MOTA	525	N	ARG	Α	136	53.014	8.261	13.018	1.00	25.65		Α
	ATOM	526	CA	ARG	Α	136	53.056	7.870	14.425	1.00	27.47		Α
25	ATOM	527	СВ	ARG			53.823	8.914	15.238	1.00	27.97		Α
	ATOM	528	CG	ARG			55.283	9.082	14.857		32.00		Α
	ATOM	529	CD	ARG			55.904	10.218	15.664		33.03		A
	ATOM	530	NE	ARG			55.602	10.073	17.084		36.11		A
•	ATOM	531	CZ	ARG			55.867	10.990	18.007		39.74		A
30	ATOM	532		ARG			56.449	12.132	17.661		40.55		A
50	ATOM	533		ARG			55.540	10.769	19.276		36.72		A
		534	C	ARG			51.667	7.709	15.036		26.38		A
	ATOM						51.516	7.121	16.106		27.06		A
	ATOM	535	0	ARG					14.360		24.77		A
25	ATOM	536	N	LEU			50.655	8.235			24.70		A.
35	MOTA	537	CA	LEU			49.294	8.162	14.870				
	ATOM	538	CB	LEU			48.483	9.363	14.371		24.52	•	A A
	ATOM	539	CG	LEU			49.050	10.760	14.662		26.67		
	ATOM	540		LEU			48.075	11.813	14.141		27.25		A
	ATOM	541		LEU			49.279	10.945	16.155		27.09		A
40	ATOM	542	C	LEU			48.592	6.868	14.473		25.20		A
	ATOM	543	, O	LEU			48.619	6.469	13.309		25.99		A
	ATOM	544	N	ASP			47.971	6.218	15.451		21.89		A
	ATOM	545	CA	ASP			47.239	4.977	15.219		21.35		A
	ATOM	546	CB	ASP	Α	138	48.124	3.761	15.523		22.14		A
45	ATOM	547	CG	ASP	А	138	47.432	2.448	15.201		24.90		A
	MOTA	548	OD1	ASP	Α	138	46.631	2.423	14.241		24.78		Α
	MOTA	549	OD2	ASP	Α	138	47.691	1.443	15.897	1.00	25,39		Α
	ATOM	550	С	ASP	Α	138	46.031	4.991	16.138	1.00	20.47		Α
	MOTA	551	0	ASP	Α	138	45.967	4.248	17.118	1.00	19.06		Α
50	ATOM	552	N	HIS	Α	139	45.075	5.852	15.810	1.00	18.27	•	. A
	ATOM	553	CA	HIS	Α	139	43.869	6.016	16.606	1.00	18.21		Α
	MOTA	554	СВ	HIS	Α	139	44.096	7.157	17.612	1.00	15.84	••	Α
	MOTA	555	CG	HIS			42.985		18.600		15.24	•-	Α
	ATOM	556		HIS			 42.884	6.964	19.900	1.00	13.97		Α
55	ATOM	557		HIS			41.791	7.943	18.280		14.74		Α
	ATOM	558		HIS			41.002	7.944	19.341		14.19		Α
	ATOM	559		HIS			41.641	7.356	20,336		14.15		A
	ATOM	560	C	HIS			42.715	6.330	15.654		18.50		
	ATOM	561	ō	HIS			42.879	7.080	14.693		20.80		A A

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	ATOM	562	N	PRO	A	140		41.527	5	.767	15.913	1.00	18.32	А
	ATOM	563	CD	PRO	Α	140		41.143	4	.984	17.100		16.71	. A
	ATOM	564	CA	PRO	A	140		40.367	6	.001	15.048		17.43	A
	ATOM	565	CB	PRO	Α	140		39.273	5	.157	15.704		16.64	A
5	ATOM	566	CG	PRO	A	140		39.643	5	.204	17.152		18.43	A
	ATOM	567	С	PRO	A	140		39.914	7	.441	14.803		18.77	A
	ATOM	568	0	PRO	Α	140		39.207	7	. 695	13.831		19.88	A
	ATOM	569	N	PHE	Α	141		40.301		.381	15.664		17.14	A
	ATOM	570	CA	PHE	Α	141		39.874	9	.767	15.477		16.42	A
10	ATOM	571	CB	PHE	Α	141		39.568	10	.422	16.836		14.60	A
	ATOM	572	CG	PHE	Α	141		38.386	· 9	.817	17.556		15.26	A
	MOTA	573	CD1	PHE	Α	141		37.335	9	.234	16.842	1.00	14.78	A
	MOTA	574		PHE				38.297	9	.880	18.942		13.70	A
	ATOM	575	CE1	PHE	Α	141		36.215	8	.727	17.502	1.00	16.94	А
15	MOTA	576	CE2	PHE				37.178	9	.375	19.615	1.00	15.75	Α
	ATOM	577	CZ	PHE	Α	141		36.135	8	.799	18.893	1.00	16.89	Α
	MOTA	578	С	PHE				40.857	10	.641	14.694	1.00	16.15	Α
	MOTA	579	0	PHE	Α	141		40.799	11	.871	14.761	1.00	17.35	А
	ATOM	580	N	PHE	Α	142		41.748	10	.011	13.941	1.00	15.88	A
20	MOTA	581	ĊA	PHE .	A	142		42.727	10	.756	13.154	1.00	17.89	A
	MOTA	582	CB	PHE .	A	142		44.115	10	.645	13.793	1.00	17.57	A
	ATOM	583	CG	PHE .				44.240	11	.371	15.103	1.00	18.74	A
	MOTA	584		PHE .				44.559		.726	15.135	1.00	17.77	A
	ATOM	585·		PHE .				43.997	10	.711	16.304	1.00	18.74	A
25	ATOM	586		PHE .				44.632		.417	16.347		15.77	A
	ATOM	587		PHE .				44.065	11	.393	17.522	1.00	17.56	A
	ATOM	588	CZ	PHE :				44.383		.747	17.542		17.14	A
	ATOM	589	С	PHE .				42.793		.231	11.729		19.12	A
	ATOM	590	0	PHE .				42.659		.030	11.504		20.01	A
30	MOTA	591	N	VAL .				42.978		.135	10.769		18.72	A
	ATOM	592	CA	VAL .				43.102		.735	9.371		18.52	Α
	ATOM	593	CB	VAL .				43.294		.961	8.440		20.66	A
	ATOM	594		VAL :				43.843		.521	7.080		21.29	A
0.5	MOTA	595		VAL				41.958		.673	8.252		22.97	A
35	MOTA	596	C	VAL				44.342		.865	9.330		18.68	A
	ATOM	597	0	VAL				45.355		.199	9.943		18.42	A
	ATOM	598	N	LYS				44.259		.745	8.623		18.30	A
	ATOM	599	CA	LYS				45.384		.824	8.535		18.78	A
40	ATOM	600	CB	LYS				44.889		.373	8.608		22.27	A
40	ATOM	601	CG	LYS				46.017		.340	8.557		29.72	A
	ATOM	602	CD	LYS A				45.491		.912	8.674 8.577		34.16 37.67	A
	ATOM ATOM	603 . 604	CE NZ	LYS A				46.631 46.138		.896 .484	8.629		39.02	A A
	ATOM	605	C	LYS A				46.136		.002	7.261		18.53	A
45	ATOM	606	0	LYS A				45.643		.314	6.200		18.18	A
43	ATOM	607	Ŋ	LEU A				47.502		.816	7.385		16.79	· A
	ATOM	608	CA	LEU A				48.411		. 900	6.251		17.45	A
	ATOM	609	CB	LEU A				49.686		. 653	6.641		18.82	A
	ATOM	610	CG	LEU A				50.734		. 902	5.549		20.23	A
50	ATOM	611		LEU A				51.836		799	6.093		18.83	A
30	ATOM	612		LEU A			•	51.317		.581	5.069		19.79	A
	ATOM	613	C	LEU A				48.739		450	5.907		19.19	A
	ATOM	614	ō	LEU A				49.451		.772	6.659		17.36	A
	ATOM	615	N	TYR A				48.215		972	4.782		17.28	A
55	ATOM	616	CA	TYR A				48.444		593	4.358		17.57	A
	ATOM	617	CB	TYR A				47.288		098	3.486		17.74	A
	ATOM	618	CG	TYR A				45.981		926	4.214		17.50	A
	ATOM	619		TYR A				45.099		995	4.377		16.50	A
	ATOM	620		TYR A				43.881		827	5.039		17.10	A
				*	-			32.002		J- '	2.005			

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	ATOM	621	CD2 T	YR A 146	45.620	2.686	4.735	1.00 18.28	A
	ATOM	622	CE2 TY	YR A 146	44.411	•			A
	MOTA	623		YR A 146		3.576		1.00 17.53	A
	ATOM	624		R A 146		3.376		1.00 20.67	A
5	ATOM	625		TR A 146	49.735	4.376	3.582	1.00 18.72	A
	MOTA	626		TR A 146	50.382			1.00 19.51	A
	MOTA	627		IE A 147	50.110		2.765	1.00 18.09	A
	ATOM	628	CA PE	IE A 147	51.307		1.952	1.00 17.20	A
	ATOM	629		IE A 147	51.007		0.783	1.00 16.77	A
10	ATOM	630		IE A 147	49.835	4.699	-0.070	1.00 17.75	A
	ATOM	631	CD1 PH	IE A 147	49.967	5.752	-0.975	1.00 16.58	A
	MOTA	632		E A 147	48.595	4.075	0.053	1.00 18.07	A
	ATOM	633		E A 147	48.886	6.178	-1.742	1.00 19.62	A
	MOTA	634		E A 147	47.503	4.492	-0.710	1.00 18.56	A
15	ATOM	635		E A 147	47.647	5.546	-1.610	1.00 19.27	A
	ATOM	636		E A 147	51.768	6.533	1.395	1.00 17.13	A
	ATOM	637	О РН	E A 147	51.045	7.528	1.452	1.00 14.43	A
	ATOM	638	N TH	R A 148	.52.981	6.534	0.854	1.00 17.12	A
	MOTA	639		R A 148	53.541	7.718	0.232	1.00 17.96	A
20	ATOM	640		R A 148	54.449	8.531	1.197	1.00 21.51	A
	ATOM	641	OG1 TH	R A 148	. 55.605	7.760	1.537	1.00 18.83	A
	ATOM	642		R A 148	53.700	8.897	2.472	1.00 19.60	A
	MOTA	643		R A 148	54.386	7.262	-0.946	1.00 20.31	А
	ATOM	644		R A 148	54.860	6.124	-0.991	1.00 18.94	Α
25	MOTA	645		E A 149	54.543	8.149	-1.916	1.00 19.16	A
	MOTA	646		E A 149	55.368	7.877	-3.073	1.00 18.01	A
	ATOM	647		E A 149	54.748	6.801	-3.989	1.00 17.23	A
	ATOM	648		E A 149	53.389	7.144	-4.544	1.00 16.88	A
20	ATOM	649	CD1 PH		53.262	7.888	-5.712	1.00 18.58	A
30	ATOM	650		E A 149	52,235	6.668	-3.927	1.00 17.31	A
	ATOM	. 651		E A 149	52.007	8.149	~6.267	1:00 19.26	A
	ATOM	652		E A 149	50.972	6.923	-4.470	1.00 19.17	A
	ATOM	653		E A 149	50.858	7.663	-5.642	1.00 19.60	A
35	ATOM	654		E A 149	55.542	9.205	-3.774	1.00 20.85	A
33	ATOM	655		E A 149	54.934	10.200	-3.376	1.00 19.76	A
	MOTA	656		N A 150	56.398	9.241	-4.782	1.00 19.79	. A
	ATOM	657		N A 150	56.636	10.481	-5.497	1.00 24.03	A
	ATOM	658		N A 150	57.659	11.347	-4.739	1.00 24.45	A
40	ATOM ATOM	659		N A 150	58.986	10.645	-4.414	1.00 26.28	· A
70	ATOM	660 661		N A 150	59.988	11.558	-3.692	1.00 29.02	A
	ATOM	662		N A 150 N A 150	60.693	12.353	-4.321	1.00 27.05	· A
	ATOM	663		N A 150	60.042	11.449	-2.365	1.00 26.47	A
	ATOM	664		N A 150	57.160	10.203	-6.885	1.00 23.88	A
45					57.673	9.118	-7.158	1.00 24.79	A
1.5	ATOM ATOM	665 666		P A 151 P A 151	56.987	11.171	-7.774	1.00 25.88	A
	ATOM	667			57.527	11.047	-9.117	1.00 26.49	A
	ATOM	668		A 151 A 151	56.437	11.126 -		1.00 24.54	A
	ATOM	669	OD1 ASP		55.544 56.005	12.336 -		1.00 24.95	A
50	ATOM	670	OD1 ASP		54.369	13.379	-9.561	1.00 22.44	A
-	ATOM	671		A 151	58.515	12.242 -		1.00 25.72	A
	ATOM	672		A 151	58.890	12.203	-9.220	1.00 28.63	A
	ATOM	673		A 151	58.934	12.780	-8.194	1.00 27.83	A
	ATOM	674		A 152	59.907	12.560 -		1.00, 29.21	A
55	ATOM	675		A 152	60.325	13.636 -		1.00 31.88	A
	ATOM	676		A 152	61.033	13.792 -		1.00 33.94	A
	ATOM	677	OD1 ASP		61.817	12.564 - 11.959 -		1.00 38.88	A
	ATOM	678	OD2 ASP		60.817	12.211 -		1.00 39.67	A
	ATOM	679		A 152	59.487			1.00 41.57	A
			- 4101	202	33.407	14.994 -	.10.012	1.00 30.90	A

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	ATOM	680	0	ASP A	152	60.316	15.735	-9.482	1.00	31.69	A
	ATOM	681	N	GLU A	•	58.207	15.322	-10.107		29.44	A
	ATOM	682	CA	GLU A		57.767	16.632	-9.646		28.69	A
	ATOM	683	CB	GLU A		56.984		-10.766		32.90	A
5	ATOM	684	CG	GLU A		57.451		-12.183		40.57	A
•	ATOM	685	CD	GLU A		56.920		-12.675		45.78	A
	ATOM	686	OE1			55.682		-12.760		48.91	A
	ATOM	687		GLU A				-12.979		48.95	A
	ATOM	688	C	GLU A		56.929	16.683	-8.372		26.43	A
10		689	0	GLU A				-7.660		25.08	A
10	ATOM					56.947	17.688				
	ATOM	690	N	LYS A		56.205	15.610	-8.069		22.39 21.43	A
	ATOM	691	CA	LYS A		55.318	15.631	-6.912			A
	ATOM	692	CB	LYS A		53.861	15.628	-7.398		20.33	. A
15	ATOM	693	CG	LYS A		53.505	16.716	-8.403		21.92	A
15	ATOM	694	CD	LYS A		52.211	16.375	-9.146		19.70	A
	MOTA	695	CE	LYS A		51.775		-10.077		20.04	A
	ATOM	696	NZ	LYS A		50.631		-10.951		19.97	A
	ATOM	697	С	LYS A		55.458	14.522	-5.881		20.43	A
	ATOM	698	0	LYS A		55.949	13.426	-6.173		21.13	A
20	ATOM	699	N	LEU A		54.985	14.832	-4.676		19.69	. A
	ATOM	700	CA	LEU A		54.950	13.900	-3.553		19.10	A
	ATOM	701	CB	LEU A		55.362	14.588	-2.252		19.65	A
	MOTA	702	CG	LEU A		56.740	15.234	-2.129		21.20	A
	ATOM	703	CD1			56.848	15.918	-0.770		23.42	· A
25	ATOM	704	CD2	LEU A	155	57.816	14.174	-2.277		23.08	A
	ATOM	705	С	LEU A		53.478	13.507	-3.427		18.87	A
	MOTA	706	0	LEU A	155	52.600	14.348	-3.620		18.61	A
	MOTA	707	N	TYR A		53.209	12.249	-3.091		15.02	A
	ATOM	708	CA	TYR A	156'	51.834	11.783	-2.934		16.29	A
30	MOTA	709	CB	TYR A	156	51.470	10.769	-4.029		14.20	A
	ATOM .	710	CG	TYR A	156	51.603	11.273	-5.449	1.00	17.29	A
	ATOM	711	CD1	TYR A	156	52.857	11.429	-6.045		16.46	A
	MOTA	712	CE1	TYR A	156	52.978	11.884	-7.360	1.00	18.68	A
	ATOM	713	CD2	TYR A	156	50.474	11.588	-6.202	1.00	16.43	A
35	ATOM	714	CE2	TYR A	156	50.583	12.048	-7.512	1.00	16.31	, A
	ATOM	715	CZ	TYR A	156	51.835	12.192	-8.083	1.00	18.17	A
	ATOM	716	OH	TYR A	156	51.941	12.651	-9.371	1.00	17.47	A
	ATOM	717	С	TYR A	156	51.657	11.108	-1.572	1.00	16.32	A
	ATOM	718	0 .	TYR A	156	52.412	10.197	-1.235	1.00	16.27	A
40	MOTA	719	N	PHE A	157	50.678	11.568	-0.792	1.00	15.47	Α
	ATOM	720	CA	PHE A	157	50.385	10.966	0.508	1.00	16.66	· A
•	ATOM	721	CB	PHE A	157	50.324	12.014	1.629	1.00	16.91	Α
	ATOM	722	CG	PHE A	157	51.631	12.708	1.907	1.00	18.96	A.
	ATOM	723	CD1	PHE A	157	52.821	12.261	1.340	1.00	20.31	A
45	ATOM	724	CD2	PHE A	157	51.664	13.829	2.732	1.00	21.12	A
	ATOM	725		PHE A		54.025	12.926	1.585	1.00	22.08	A
	ATOM	726		PHE A		52.865	14.500	2.982		22.18	A
	ATOM	727	CZ	PHE A	157	54.045	14.045	2.405		21.27	A
	ATOM	728	C	PHE A		49.016	10.308	0.404	1.00	16.52	A
50	ATOM	729	Ō.	PHE A		48.029	10.979	0.110		17.32	A
•	ATOM	730	N	GLY A		48.953	9.002	0.644		15.97	A
	ATOM	731	CA	GLY A		47.684	8.299	0.572		16.13	A
	ATOM	732	C	GLY A		47.000	8.383	1.920		14.94	A
	ATOM	733	Ö	GLY A		47.445	7.756			16.28	A
55	ATOM	734	N	LEU A		45.915	9.145	1.989		13.50	A
23	ATOM	735	CA	LEU A		45.191	9.340	3.241		15.20	A
	ATOM	736	CB	LEU A		45.031	10.835	3.517		14.20	A
	ATOM	737	CG	LEU A		46.270	11.726	3.385		19.00	A
	ATOM	738		LEU A		45.847	13.188	3.477		17.12	A
	ALON	, 50	CDI	TO A	100	40.047	10.100				

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	ATOM	739	CD2	LEU A	159	47.275	11.390	4.471	1.00 1	4.71	А
	ATOM	740	С	LEU A	159	43.809	8.716	3.232	1.00 1		A
	ATOM	741	0	LEU A	159	43.232	8.472	2.177	1.00 1		A
	ATOM	742	N	SER A	160	43.268	8.469	4.418	1.00 1		A
5	ATOM	743	CA	SER A	160	41.932	7.917	4.498	1.00 1		A
	ATOM	744	CB	SER A	160	41.566	7.582	5.949	1.00 2		A
	ATOM	745	OG	SER A		41.901	8.629	6.833	1.00 2		A
	ATOM	746	C	SER A		40.987	8.968	3.924	1.00 2		A
	ATOM	747	ō	SER A		41.213	10.173	4.062	1.00 1		A
10	ATOM	748	N	TYR A		39.945	8.508	3.250	1.00 1		A
	ATOM	749	CA	TYR A		38.975	9.406	2.644	1.00 20		A
	ATOM	750	СВ	TYR A		38.471	8.785	1.332	1.00 20		A
	ATOM .	751	CG	TYR A		37.314	9.502	0.666	1.00 20		A
	ATOM	752		TYR A		37.222	10.895	0.682	1.00 18		A
15	ATOM	753		TYR A		36.180	11.557	0.029	1.00 2		A.
13	ATOM	754		TYR A		36.333	8.784	-0.020	1.00 20		A
	ATOM	755		TYR A		35.287	9.436	-0.678	1.00 2		A
•	ATOM	756	CZ	TYR A		35.218	10.822	-0.648	1.00 22		. A
	ATOM	757	OH	TYR A		34.194	11.471	-1.298	1.00 23		A
20	ATOM	758	C	TYR A		37.812	9.681	3.598	1.00 2		Ā
20	ATOM	759	Ö	TYR A		36.959	8.819	3.810	1.00 19		A
	ATOM	760	N	ALA A		37.791	10.880	4.178	1.00 19		A
	ATOM	761	CA	ALA A		36.721	11.271	5.099	1.00 23		A
	ATOM	762	CB	ALA A		37.187	12.419	6.002	1.00 19		A
25	ATOM	763	C	·ALA A		35.542	11.712	4.238	1.00 22		A
23	ATOM	764	Ö	ALA A		35.436	12.875	3.860	1.00 20		· A
-	MOTA	765	N	LYS A		34.653	10.769	3.945	1.00 23		A
	ATOM	766	CA	LYS A		33.503	11.017	3.080	1.00 2		A
	ATOM	767	СВ	LYS A		32.663	9.741	2.963	1.00 29		A
30	ATOM	768	CG	LYS A		33.455	8.524	2.515	1.00 3		A
	ATOM	769	CD	LYS A		32.556	7.310	2.321	1.00 42		A
	ATOM	770	CE	LYS A		33.373	6.034	2.185	1.00 44	1.48	Α
	ATOM	771	NZ	LYS A		34.143	5.735	3.430	1.00 44	1.88	A
	ATOM	772	С	LYS A	163	32.581	12.186	3.411	1.00 29	5.78	A
35	ATOM	773	0	LYS A	163	32.103	12.863	2.506	1.00 26	5.53	Α
	ATOM	774	N	ASN A	164	32.327	12.441	4.689	1.00 24	1.57	A
	ATOM	775	CA	ASN A	164	31.420	13.522	5.033	1.00 23	3.77	A
	ATOM	776	CB	ASN A	164	30.610	13.129	6.265	1.00 25	5.02	A
	ATOM	777	CG ·	ASN A	164	29.537	12.101	5.932	1.00 27	7.54	A
40	ATOM	778		ASN A		28.772	12.281	4.983	1.00 28		A
	ATOM	779	ND2	ASN A	164	29.475	11.024	6.704	1.00 2		A
	ATOM	780	С	ASN A	164	31.999	14.931	5.169	1.00 24		A
	ATOM	781	0	ASN A	164	31.306	15.856	5.589	1.00 23		A
	MOTA	782	N	GLY A		33.262	15.097	4.795	1.00 23		A
45	MOTA	783	CA	GLY A		33.873	16.414	4.836	1.00 24		A
	ATOM	784	С	GLY A		34.191	17.043	6.181	1.00 23		A
	MOTA	785	0	GLY A		34.380	16.352	7.177	1.00 23		A
	ATOM	786	N	GLU A		34.234	18.373	6.186	1.00 23		A
	MOTA	787	CA	GLU A		34.563	19.176	7.362	1:00 24		A
50	ATOM	788	CB	GLU A	166	35.055	20.558	6.913	1.00 25		A
	ATOM	789	CG	GLU A		36.419	20.569	6.229	1.00 26		A
	ATOM	790	CD	GLU A		36.699	21.889	5.517	1.00 30		Α
	ATOM	791		GLU A		36.081	22.906	5.889	1.00 29		A
	ATOM	792		GLU A		37.544	21.916	4.596	1.00 30		A
55	ATOM	793	С	GLU A		33.436	19.372	8.369	1.00 24		A
	ATOM	794	0	GLU A		32.279	19.541	8.001	1.00 22		A
	ATOM	795	N	LEU A		33.791	19.370	9.649	1.00 22		A
	ATOM	796	CA	LEU A		32.813	19.581	10.707	1.00 22		A
	ATOM	797	CB	LEU A	167	33.497	19.481	12.073	1.00 22	2.32	A

	MOTA	798	CG	א ונים.ז	167		22 706	10 022	12 200			
	ATOM	799		LEU A				19.923	13.306		22.04	A
	ATOM	800					31.454		13.463		19.66	A
	ATOM			LEU A			33.597		14.537		21.17	A
5		801	_	LEU A			32.193		10.529		23.49	A
3	ATOM .	802	-	LEU A			31.047	-	10.907	. 1.00	23.56	A
	ATOM	803	N	LEU A	168		32.960	21.887	9.948		24.25	A
	MOTA	804	CA	LEU A			32.473	23.245	9.722		26.64	A
	ATOM	805	CB	LEU A	168		33.560	24.099	9.066		25.62	A
	ATOM	806	CG	LEU A	168		33.198	25.546	8.707		27.34	A
10	ATOM	807		LEU A			32.718	26.296	9.946		26.42	A
	ATOM	808		LEU A			34.418	26.238	8.119		26.74	
	ATOM	809		LEU A			31.234	23.218	8.829			A
	ATOM	810		LEU A			30.297	23.210	9.030		27.13	A
	ATOM	811		LYS A							26.01	Α
15	ATOM	812		LYS A			31.233	22.320	7.848		26.41	A
15	ATOM	813					30.106	22.210	6.934		27.70	A
	ATOM			LYS A			30.324	21.064	5.945		30.49	A
		814		LYS A			29.151	20.854	4.993	1.00	32.47	Α
	ATOM	815		LYS A			29.407	19.728	3.998	1.00	35.98	Α
00	ATOM	816		LYS A		2	29.462	18.372	4.683	1.00	38.53	A
20	ATOM	817		LYS A		2	29.622	17.263	3.702	1.00	41.00	Α
	MOTA	818		LYS A			28.801	21.985	7.682		28.12	A
	MOTA	819	0	LYS A	169	2	27.785	22.608	. 7.371		28.08	A
	ATOM	820	N	TYR A	170	2	8.826	21.094	8.668		26.53	A
	ATOM	821	CA '	TYR A	170	2	7.624	20.791	9.434		26.95	A
25	MOTA	822		TYR A			7.810	19.476	10.193		25.03	·A
	ATOM	823		TYR A			7.898	18.300	9.251		26.65	
	ATOM	824		TYR A			6.745	17.661	8.790		28.27	A
	ATOM	825		TYR A			6.814	16.642				A
	ATOM	826		TYR A			9.127		7.839		26.85	A
30	ATOM	827		TYR A				17.884	8.742		27.83	. A
••	ATOM	828	CZ :	TYR A	170		9.209	16.869	7.792		27.19	. А
	ATOM	829					8.049	16.254	7.343		30.02	A
	ATOM			ryr a			8.130	15.268	6.382		29.23	A
		830		FYR A			7.229	21.918	10.376		27.59	Α
25	ATOM -	831		TYR A			6.045	22.122	10.642	1.00	29.25	A
35	ATOM	832		LLE A		2	8.208	22.660	10.882	1.00	28.16	A
	ATOM	833		ILE A		2	7.883	23.770	11.763	1.00	29.03	· A
	ATOM	834		LE A		. 2	9.151	24.435	12.337	1.00	27.51	A
	ATOM	835		LE A		2	8.773	25.705	13.084		27.97	A
	ATOM	836	CG1 I	LE A	171	2	9.872	23.458	13.272		26.70	A
40	MOTA	837	CD1 I	LE A	171	3	1.163	23.996	13.856		24.07	A
	ATOM	838		LE A			7.094	24.796	10.944		31.41	A
	ATOM	839		LE A			6.088		11.407		31.69	
	ATOM	840		RG A			7.546	25.047	9.719		33.21	A
	ATOM	841		RG A 1			6.874	26.000	8.844			A
45	ATOM	842		RG A			7.734				36.54	A
-	ATOM	843						26.314	7.616		37.73	A
-	ATOM	844		RG A 1			9.057	27.011	7.912		41.65	A
				RG A 1			9.708	27.492	6.616		45.29	A
	MOTA	845		RG A 1			1.037	28.070	6.812		48.51	A
50	ATOM	846		RG A 1			1.314	29.059	7.658	1.00	51.53	A
50	ATOM	847		RG A 1		30	0.355	29.593	8.406	1.00	53.75	A
	ATOM	848	NH2 A	RG A 1	.72	32	2.553	29.526	7.748	1.00	51.21	A
	ATOM	849		RG A 1		25	5.528	25.459	8.378	1.00	37.67	Α
	ATOM	850		RG A 1		24	1.550	26.200	8.288	1.00		A
	ATOM	851		YS A 1			.481	24.163	8.092	1.00		A
55	ATOM	852		YS A 1			.259	23.528	7.619	1.00		A
	ATOM	853		YS A 1			.523	22.061	7.272	1.00		
	ATOM	854		YS A 1			3.279	21.298				A
	ATOM	855		YS A 1				19.808	6.830	1.00		A
	ATOM	856		YS A 1					6.653	1.00		A
		000	υυ <u>μ</u>	-> M I	, ,	24	.477	19.530	5.469	1.00	52.63	A

	ATOM	857	NZ	LYS	Α	173	23.855	19.894	4.160	1 00	54.61		70
•	ATOM	858	C			173	23.089	23.608	8.595		39.30		A
	ATOM	859	Ö			173							A
							21.981	23.960	8.201		39.62		Α
_	ATOM	860	N			174	23320	23.282	9.863		37.96		Α
5	ATOM	861	CA			174	22.229	23.314	10.833	1.00	37.36		Α
	ATOM	862	CB	ILE	Α	174	22.159	21.998	11.652	1.00	37.44		Α
	MOTA	863	CG2	: ILE	A	174	22.058	20.802	10.709	1.00	38.37		Α
	ATOM	864	CG1	ILE	A	174	23.397	21.850	12.532		37.25		Α
	ATOM	865	CD1			174	23.355	20.620	13.418		36.85		A
10	ATOM	866	C			174	22.259	24.492	11.801		36.71		
10	ATOM	867	Ö			174							A
							21.448	24.556	12.724		38.05		Α
	ATOM	868	N			175	23.185	25.423	11.592		35.48		Α
•	ATOM	869	CA			175	23.265	26.585	12.462	1.00	35.29		Α
	MOTA	870	С			175	24.053	26.360	13.737	1.00	35.06		Α
15	ATOM	871	0	GLY	Α	175	25.066	27.019	13.970	1.00	37.46		A
	ATOM	872	N	SER	Α	176	23.581	25.441	14.571	1.00	33.94		A
	ATOM	873	CA	SER	Α	176	24.253		15.822		32.84		A
	ATOM	874	CB			176	23.938	26.155	16.901		33.54		A
	ATOM	875	OG			176	22.599						
20	ATOM	876						26.056	17.347		34.86		A
			С			176	23.796	23.731	16.276		32.34		A
	ATOM	877	0			176	22.726	23.263	15.884		32.82		A
	ATOM	878	N			177	24.609	23.085	17.103	1.00	29.39		Α
	ATOM	879	CA	PHE	Α	177	24.313	21.743	17.597	1.00	27.20		A.
	ATOM	880	CB	PHE	Α	177	25.621	20.989	17.865	1.00	26.39		Α
25	ATOM	881	CG	PHE	Α	177	26.372	20.585	16.622	1.00	26.18		A
	ATOM	882	CD1	PHE	Α	177	26.210	21.277	15.426		25.30		A
	ATOM	883		PHE			27.266	19.516	16.662		26.05		A
	ATOM	884		PHE			26.923	20.912	14.290		26.59		A
•	ATOM	885	CE2				27.986						
30	ATOM	886	CZ					19.143	15.532		26.06		A
30						177	27.815	19.841	14.343		25.42		A
	ATOM	887	C			177	23.500	21.752	18.884		27.00		Α
	ATOM	888	0	PHE	A	177	23.704	22.610	19.747	1.00	26.48		A
	ATOM	889	N	ASP	Α	178	22.578	20.802	19.022	1.00	26.70		A
	MOTA	890	CA	ASP	A	178	21.816	20.729	20.260	1.00	26.35		Α
35	ATOM	891	CB	ASP	Α	178	20.621	19.773	20.142	1.00	29.90		Α
	ATOM	892	CG	ASP			21.020	18.372	19.720		32.28		A
	ATOM	893		ASP			22.157	17.949	20.014		35.21		A
	ATOM	894		ASP			20.179	17.683	19.105		34.79		A
	ATOM	895	C.	ASP			22.810	20.228	21.311				
40	ATOM	896	Ö	ASP							25.03		A
70							23.974	19.968	20.992		21.24		A
	MOTA	897	N	GLU			22.361	20.083	22.552		23.60		Α
	ATOM	898	CA	GLU			23.247	19.644	23.619	1.00	25.18		Α
	ATOM	899	CB	GLU	Α	179	22.542	19.770	24.971	1.00	27.60		Α
	ATOM	900	CG	GLU	Α	179	23.324	19.176	26.130	1.00	32.58		A
45	ATOM	901	CĎ	GLÜ	Α	179	22.997	19.845	27.449	1.00	35.82		Α
	ATOM	902	OE1	GLU	А	179	21.825	20.224	27.645		35.95		Α
	ATOM -	903		GLU			23.912	19.984	28.291		38.19		A
	ATOM	904	C	GLU			23.808	18.235	23.450		24.08		
	ATOM	905	0	GLU			24.977					•	Α.
50	ATOM							17.989	23.756		22.79		A.
50		906	N	THR			22.983	17.316	22.961		23.36		Α
	ATOM	907	CA	THR			23.412	15.935	22.761		22.15		Α
	ATOM	908	CB	THR			22.224	15.054	22.320	1.00	23.77		Α
	MOTA	909	OG1	THR	Α	180	21.222	15.075	23.341	1.00	26.37		Α
	MOTA	910	CG2	THR	A	180	22.670	13.616	22.088		22.66		A
55	ATOM	911	С	THR			24.533	15.830	21.724		22.01		A
	ATOM	912	Õ	THR			25.533	15.141	21.944		19.87		A
	ATOM	913	N	CYS			24.365	16.511	20.596		21.21		
	ATOM	914	CA	CYS			25.372						A
-								16.480	19.541		22.22		A
	ATOM	915	CB	CYS	н	ToT	24.800	17.065	18.250	1.00	24.62		A

ATOM 916 SG CVS A 181														
ATOM 918 O CYS A 181 27.746 16.827 19.608 1.00 23.95 ATOM 920 CA THR A 182 27.606 19.103 21.161 1.00 21.49 ATOM 921 CB THR A 182 27.606 19.103 21.161 1.00 21.49 ATOM 922 CG THR A 182 27.606 19.103 21.161 1.00 21.49 ATOM 923 CG2 THR A 182 28.379 21.046 22.565 1.00 18.36 ATOM 924 C THR A 182 28.379 21.046 22.565 1.00 18.36 ATOM 925 C THR A 182 28.379 21.046 22.565 1.00 18.36 ATOM 925 O THR A 182 29.669 18.090 21.894 1.00 19.95 ATOM 926 N ARG A 183 29.669 18.090 21.894 1.00 19.95 ATOM 927 CA ARG A 183 28.468 16.723 23.996 1.00 19.39 ATOM 928 CG ARG A 183 27.051 14.571 26.925 1.00 19.39 ATOM 929 CG ARG A 183 27.051 14.571 26.925 1.00 21.19 ATOM 929 CG ARG A 183 27.051 14.571 26.925 1.00 21.19 ATOM 930 CD ARG A 183 27.021 14.571 26.925 1.00 21.19 ATOM 931 NE ARG A 183 26.605 15.642 27.824 1.00 19.46 ATOM 933 NH1 ARG A 183 25.496 16.362 27.679 1.00 21.45 ATOM 933 NH1 ARG A 183 25.496 16.362 27.679 1.00 20.45 ATOM 935 C ARG A 183 25.244 17.338 28.539 1.00 17.11 ATOM 936 O ARG A 183 30.383 15.333 23.573 1.00 19.97 ATOM 937 N PHE A 184 28.158 13.078 20.577 23.302 1.00 20.45 ATOM 937 N PHE A 184 28.158 13.078 20.764 1.00 19.97 ATOM 937 N PHE A 184 28.158 13.078 20.764 1.00 22.67 ATOM 930 CD PHE A 184 28.158 13.078 20.764 1.00 22.67 ATOM 930 CD PHE A 184 28.717 10.630 20.754 1.00 22.67 ATOM 940 CC PHE A 184 29.104 13.746 21.722 1.00 18.04 ATOM 940 CC PHE A 184 29.104 13.746 21.722 1.00 18.04 ATOM 940 CC PHE A 184 29.107 19.49 18.850 1.00 19.97 ATOM 940 CC PHE A 184 29.107 19.49 18.850 1.00 19.97 ATOM 940 CC PHE A 184 29.107 19.49 18.850 1.00 19.37 ATOM 940 CC PHE A 184 29.910 9.613 18.928 1.00 22.97 ATOM 940 CC PHE A 184 29.910 9.613 18.928 1.00 22.97 ATOM 940 CC PHE A 184 29.910 9.613 18.928 1.00 12.05 ATOM 940 CC PHE A 184 29.910 9.613 18.928 1.00 12.05 ATOM 940 CC PHE A 184 29.910 9.613 18.928 1.00 12.05 ATOM 940 CC PHE A 184 29.910 19.613 18.928 1.00 12.05 ATOM 940 CC PHE A 184 29.910 9.613 18.928 1.00 12.05 ATOM 940 CC PHE A 184 29.910 10.6103 10.05 ATOM 940 CC PHE A 184 29.910 10.6103 10.05 ATOM 940 CC PHE A 184 29.		MOTA	916	SG .				23.435	16.080	17.560	1.00	29.50		Α
ATOM		ATOM	917	С	CYS	A	181	26.633	17.232	19.954				A
S		ATOM	918	0	CYS	Α	181	27.746	16.827	19.608	1.00	23.95		A
ATOM		ATOM	919	N	THR	Α	182	26.463	18.325	20.695	1.00	22.76		A
ATOM	5	ATOM	920	CA	THR	Α	182	27.606	19.103	21.161	1.00	21.49		Α
ATOM		ATOM	921	CB	THR	Α	182	27.167	20.346	21.978	1.00	21.37		A
ATOM		ATOM	922	OG1	THR	Α	182	26.459	21.262		1.00	22.50		Α
10		ATOM	923	CG2	THR	Α	182	28.379	21.046	22.565	1.00	18.36		A
ATOM 926 N ARG A 183 27.799 17.602 23.050 1.00 18.97 ATOM 927 CA ARG A 183 28.468 16.723 23.996 1.00 19.46 ATOM 928 CB ARG A 183 28.468 16.723 23.996 1.00 19.46 ATOM 929 CG ARG A 183 28.030 15.062 25.887 1.00 19.46 ATOM 931 NE ARG A 183 27.021 14.571 26.925 1.00 21.19 ATOM 931 NE ARG A 183 26.605 15.642 27.824 1.00 19.46 ATOM 932 CZ ARG A 183 26.605 15.642 27.824 1.00 19.46 ATOM 933 NH ARG A 183 26.605 15.642 27.679 1.00 20.19 ATOM 934 NE ARG A 183 25.496 16.362 27.679 1.00 20.02 ATOM 934 NE ARG A 183 25.246 16.123 26.666 1.00 19.81 ATOM 935 C ARG A 183 25.224 17.338 28.539 1.00 17.11 20 ATOM 936 C ARG A 183 30.383 15.333 23.573 1.00 19.97 ATOM 937 N PHE A 184 28.520 14.871 22.409 1.00 19.97 ATOM 938 CA PHE A 184 28.520 14.871 22.409 1.00 19.97 ATOM 939 CB PHE A 184 28.158 13.078 20.764 1.00 22.67 ATOM 940 CC PHE A 184 28.719 11.857 20.098 1.00 22.67 ATOM 941 CD1 PHE A 184 28.317 10.630 20.754 1.00 22.97 ATOM 942 CD2 PHE A 184 29.318 13.078 20.764 1.00 22.97 ATOM 943 CEI PHE A 184 29.308 9.510 20.176 1.00 23.53 ATOM 944 CC2 PHE A 184 29.308 9.510 20.176 1.00 23.53 ATOM 945 CC PHE A 184 29.930 9.510 20.176 1.00 23.53 ATOM 946 C PHE A 184 29.915 10.833 18.263 1.00 24.11 30 ATOM 947 O PHE A 184 30.403 14.127 20.941 1.00 17.99 ATOM 948 N TYR A 185 30.929 15.110 20.056 1.00 15.73 ATOM 949 CA TYR A 185 30.929 16.413 18.928 1.00 22.97 ATOM 940 CE TYR A 185 30.929 16.413 18.111 1.00 17.33 ATOM 950 CE TYR A 185 30.929 16.413 18.111 1.00 17.33 ATOM 950 CE TYR A 185 30.929 16.413 18.111 1.00 17.33 ATOM 950 CE TYR A 185 30.929 16.413 18.111 1.00 17.36 ATOM 950 CE TYR A 185 30.929 16.413 18.211 1.00 16.62 ATOM 950 CE TYR A 185 30.929 16.413 18.201 1.00 18.14 ATOM 950 CE TYR A 185 30.929 16.413 18.201 1.00 16.03 ATOM 950 CE TYR A 185 30.929 16.413 18.011 1.00 17.99 ATOM 950 CE TYR A 185 30.929 16.413 1.00 16.16 1.00 16.63 ATOM 960 CE TYR A 185 30.929 16.413 1.00 16.16 1.00 16.63 ATOM 960 CE TYR A 185 30.990 16.414 17.00 16.03 ATOM 960 CE TYR A 185 30.990 16.00 16.16 10.00 16.63 ATOM 960 CE TYR A 186 33.554 18.403 22.823 1.00		MOTA	924	С	THR	Α	182	28.454	18.215	22.071	1.00	21.48		Α
ATOM 927	10	MOTA	925	0	THR	Α	182	29.669	18.090	21.894	1.00	19.95		A
ATOM 928 CB ARG A 183		MOTA	926	N	ARG	A	183	27.798	17.602	23.050				Α
ATOM 929 CG ARG A 183 28.030 15.062 25.887 1.00 18.77 ATOM 931 NE ARG A 183 27.021 14.571 26.225 1.00 21.19 ATOM 932 CZ ARG A 183 25.496 16.362 27.824 1.00 19.46 ATOM 933 NH1 ARG A 183 25.496 16.362 27.824 1.00 19.46 ATOM 934 NH2 ARG A 183 25.496 16.362 27.824 1.00 19.46 ATOM 935 C ARG A 183 25.224 17.338 28.539 1.00 17.11 20 ATOM 936 C ARG A 183 29.206 15.577 23.302 1.00 20.02 ATOM 937 N PHE A 184 28.520 14.871 22.409 1.00 19.24 ATOM 938 CA PHE A 184 28.158 13.078 20.764 1.00 19.24 ATOM 939 CB PHE A 184 28.158 13.078 20.764 1.00 22.07 ATOM 930 CB PHE A 184 28.158 13.078 20.764 1.00 22.07 ATOM 940 CG PHE A 184 28.719 11.857 20.098 1.00 22.67 ATOM 941 CD1 PHE A 184 28.910 18.850 1.00 19.97 ATOM 942 CD2 PHE A 184 29.911 11.949 18.850 1.00 19.97 ATOM 943 CE1 PHE A 184 29.911 11.949 18.850 1.00 19.97 ATOM 945 CZ PHE A 184 29.915 10.833 18.263 1.00 22.176 ATOM 946 C PHE A 184 29.910 9.613 18.928 1.00 22.97 ATOM 947 O PHE A 184 29.910 10.833 18.263 1.00 22.97 ATOM 948 N TYR A 185 30.292 15.110 20.056 1.00 15.73 ATOM 948 N TYR A 185 30.292 15.110 20.056 1.00 15.73 ATOM 949 CA TYR A 185 30.922 15.110 20.056 1.00 15.73 ATOM 950 CB TYR A 185 30.992 14.809 19.265 1.00 15.73 ATOM 951 CG TYR A 185 30.992 16.413 18.111 1.00 17.33 ATOM 955 CZ TYR A 185 30.590 13.952 15.232 1.00 18.18 40 ATOM 956 CZ TYR A 185 30.590 13.952 15.232 1.00 18.18 41 ATOM 957 CD TYR A 185 30.590 13.952 15.232 1.00 18.18 42 ATOM 956 CZ TYR A 185 30.590 13.952 15.232 1.00 18.18 43 ATOM 957 CD TYR A 185 30.590 13.952 15.232 1.00 18.18 44 ATOM 958 CZ TYR A 185 30.590 13.952 15.232 1.00 18.18 45 ATOM 956 CZ TYR A 185 30.590 13.952 15.232 1.00 18.18 46 ATOM 957 CD TYR A 185 30.590 13.952 15.232 1.00 18.18 47 ATOM 958 CZ TYR A 185 30.590 13.952 15.232 1.00 18.18 48 ATOM 958 CZ TYR A 185 30.590 13.952 15.232 1.00 18.18 49 ATOM 958 CZ TYR A 185 30.590 13.952 15.232 1.00 18.18 40 ATOM 957 CD TYR A 185 30.590 13.952 15.232 1.00 18.18 41 ATOM 958 CZ TYR A 185 30.590 13.952 15.232 1.00 18.18 41 ATOM 957 CD TYR A 185 30.590 12.955 14.218 1.00 17.69 41 ATOM 968 CA		MOTA	927	CA	ARG	Α	183	28.468	16.723	23.996	1.00	19.39		Α
ATOM		MOTA	928	CB	ARG	A	183	27.455	16.140	24.984	1.00	19.46		A
ATOM		ATOM	929	CG	ARG	Α	183	28.030	15.062					Α
ATOM	15	MOTA	930	CD	ARG	Α	183	27.021	14.571	26.925	1.00	21.19		A
ATOM 932 CZ ARG A 183 25.496 16.362 27.679 1.00 20.45 ATOM 933 NH1 ARG A 183 22.224 17.338 28.539 1.00 17.11 20 ATOM 935 C ARG A 183 25.224 17.338 28.539 1.00 17.11 20 ATOM 936 O ARG A 183 25.224 17.338 28.539 1.00 17.11 20 ATOM 936 O ARG A 183 29.206 15.577 23.302 1.00 20.02 ATOM 937 N PHE A 184 28.520 14.671 22.409 1.00 19.97 ATOM 938 CA PHE A 184 28.520 14.671 22.409 1.00 19.97 ATOM 938 CA PHE A 184 28.520 14.671 22.409 1.00 18.04 ATOM 938 CB PHE A 184 28.719 11.857 20.098 1.00 22.05 ATOM 940 CG PHE A 184 28.717 10.630 20.754 1.00 22.97 ATOM 942 CD2 PHE A 184 29.317 11.949 18.850 1.00 19.97 ATOM 942 CD2 PHE A 184 29.317 11.949 18.850 1.00 19.97 ATOM 942 CD2 PHE A 184 29.317 11.949 18.850 1.00 19.97 ATOM 942 CD2 PHE A 184 29.930 9.510 20.176 1.00 22.97 ATOM 944 CE2 PHE A 184 29.930 9.510 20.176 1.00 22.97 ATOM 945 CZ PHE A 184 29.915 10.633 18.263 1.00 22.197 ATOM 945 CZ PHE A 184 29.915 10.633 18.263 1.00 22.197 ATOM 947 O PHE A 184 29.915 10.633 18.263 1.00 22.197 ATOM 947 O PHE A 184 30.403 14.127 20.941 1.00 17.99 ATOM 948 N TYR A 185 30.292 15.110 20.056 1.00 15.73 ATOM 945 CZ PHE A 184 30.403 14.127 20.941 1.00 17.93 ATOM 949 CA TYR A 185 30.292 15.110 20.056 1.00 15.73 ATOM 950 CB TYR A 185 30.364 15.584 17.015 1.00 15.73 ATOM 951 CG TYR A 185 30.364 15.584 17.015 1.00 16.53 ATOM 952 CD1 TYR A 185 30.364 15.584 17.015 1.00 16.33 ATOM 953 CE1 TYR A 185 30.364 15.584 17.015 1.00 16.53 ATOM 955 CE2 TYR A 185 30.364 15.584 17.015 1.00 16.53 ATOM 957 CH TYR A 185 30.364 15.584 17.015 1.00 16.53 ATOM 957 CH TYR A 185 30.364 15.584 17.015 1.00 16.53 ATOM 957 CH TYR A 185 30.364 15.584 17.015 1.00 16.53 ATOM 958 CC TYR A 185 30.590 13.952 15.232 1.00 18.14 ATOM 957 CH TYR A 185 30.590 13.952 15.232 1.00 18.14 ATOM 958 CC TYR A 185 30.590 13.952 15.232 1.00 18.15 ATOM 950 CH TYR A 185 30.590 13.952 15.232 1.00 18.54 ATOM 957 CH TYR A 185 30.590 13.952 15.232 1.00 18.54 ATOM 958 CC TYR A 185 30.590 13.952 15.232 1.00 18.54 ATOM 958 CC TYR A 185 30.590 13.952 15.232 1.00 18.54 ATOM 958 CC TYR A 185 30.590 13.952		ATOM	931	NE	ARG	A	183	26.605	15.642					A
ATOM 933 NH1 ARG A 183		ATOM	932	CZ.	ARG	A	183	25.496	16.362					Α
ATOM		ATOM	933	NH1	ARG	Α	183	24.672						A
ATOM		ATOM	934	NH2	ARG	Α	183	25.224						Α
ATOM 936 O ARG A 183 30.383 15.333 23.573 1.00 19.97 ATOM 937 N PHE A 184 28.520 14.871 22.009 1.00 19.24 ATOM 938 CA PHE A 184 28.158 13.078 20.0764 1.00 22.67 ATOM 939 CB PHE A 184 28.158 13.078 20.098 1.00 22.67 ATOM 941 CD1 PHE A 184 28.717 10.630 20.754 1.00 22.97 ATOM 942 CD2 PHE A 184 29.317 11.949 18.850 1.00 19.97 ATOM 943 CE1 PHE A 184 29.317 11.949 18.850 1.00 19.97 ATOM 944 CE2 PHE A 184 29.915 10.833 18.263 1.00 24.11 30 ATOM 945 CZ PHE A 184 29.915 10.833 18.263 1.00 24.11 31 ATOM 946 C PHE A 184 29.915 10.833 18.928 1.00 22.97 ATOM 947 O PHE A 184 30.403 14.127 20.941 1.00 17.99 ATOM 948 N TYR A 185 30.292 15.110 20.056 1.00 15.73 ATOM 949 CA TYR A 185 30.992 15.110 20.056 1.00 15.73 ATOM 950 CB TYR A 185 30.992 16.413 18.111 1.00 17.33 ATOM 951 CG TYR A 185 30.992 16.413 18.111 1.00 17.33 ATOM 952 CD1 TYR A 185 30.992 16.413 18.111 1.00 17.33 ATOM 954 CD2 TYR A 185 30.992 16.413 18.111 1.00 17.33 ATOM 955 CE TYR A 185 30.992 16.413 18.111 1.00 17.33 ATOM 955 CD TYR A 185 30.992 16.413 18.111 1.00 17.33 ATOM 955 CD TYR A 185 30.590 13.952 15.232 1.00 18.18 ATOM 956 CD TYR A 185 30.590 13.952 15.232 1.00 18.18 ATOM 957 CH TYR A 185 30.590 13.952 15.232 1.00 18.18 ATOM 958 C TYR A 185 30.590 13.952 15.232 1.00 18.18 ATOM 950 CD TYR A 185 30.590 13.952 15.232 1.00 18.18 ATOM 951 CG TYR A 185 30.590 13.952 15.232 1.00 18.18 ATOM 956 CZ TYR A 185 30.590 13.952 15.232 1.00 18.18 ATOM 957 CH TYR A 185 32.544 16.952 20.00 18.19 ATOM 958 C TYR A 185 32.544 16.952 20.00 31.00 15.79 ATOM 959 O TYR A 185 32.559 18.403 23.094 1.00 15.68 ATOM 960 O THR A 186 33.720 16.015 19.766 1.00 17.69 ATOM 961 CA THR A 186 33.954 16.375 22.680 1.00 13.57 ATOM 962 CB THR A 186 33.954 16.375 22.680 1.00 13.57 ATOM 963 CA THR A 186 33.954 16.375 22.680 1.00 13.57 ATOM 960 C THR A 186 33.954 16.375 22.680 1.00 14.68 ATOM 960 C THR A 186 33.954 16.375 22.680 1.00 14.68 ATOM 960 C THR A 186 33.954 16.375 22.680 1.00 14.68 ATOM 960 C THR A 186 33.954 16.375 22.680 1.00 15.59 ATOM 960 C THR A 186 33.954 16.375 22.680 1.00 14.74 A	20	ATOM	935	С	ARG	Α	183	29.206						A
ATOM 937 N PHE A 184 28.520 14.871 22.409 1.00 19.24 ATOM 938 CB PHE A 184 29.144 13.746 21.722 1.00 18.04 ATOM 939 CB PHE A 184 28.158 13.078 20.764 1.00 21.05 21.05 ATOM 940 CG PHE A 184 28.719 11.857 20.098 1.00 22.67 ATOM 941 CD1 PHE A 184 28.719 11.857 20.098 1.00 22.67 ATOM 942 CD2 PHE A 184 29.317 11.949 18.850 1.00 19.97 ATOM 942 CD2 PHE A 184 29.317 11.949 18.850 1.00 19.97 ATOM 945 CE2 PHE A 184 29.308 9.510 20.176 1.00 23.53 ATOM 945 CE2 PHE A 184 29.910 9.613 18.228 1.00 22.97 ATOM 945 CZ PHE A 184 29.910 9.613 18.228 1.00 22.97 ATOM 946 C PHE A 184 29.910 9.613 18.228 1.00 22.97 ATOM 947 O PHE A 184 30.403 14.127 20.941 1.00 17.99 ATOM 947 O PHE A 184 30.403 14.127 20.941 1.00 17.99 ATOM 947 O PHE A 184 30.403 14.127 20.941 1.00 17.99 ATOM 947 O PHE A 184 30.403 14.127 20.941 1.00 15.73 ATOM 948 N TYR A 185 30.292 15.110 20.056 1.00 15.73 ATOM 950 CB TYR A 185 30.992 16.413 18.111 1.00 17.33 ATOM 951 CG TYR A 185 30.992 16.413 18.111 1.00 17.33 ATOM 951 CG TYR A 185 30.992 16.413 18.111 1.00 17.33 ATOM 953 CE1 TYR A 185 30.590 13.952 15.232 1.00 18.12 ATOM 954 CD2 TYR A 185 30.590 13.952 15.232 1.00 18.12 ATOM 955 CE2 TYR A 185 30.590 13.952 15.232 1.00 18.12 ATOM 955 CD2 TYR A 185 30.590 13.952 15.232 1.00 18.12 ATOM 957 OH TYR A 185 30.590 13.952 15.232 1.00 18.12 ATOM 957 OH TYR A 185 30.590 13.952 15.232 1.00 18.12 ATOM 957 OH TYR A 185 30.590 13.952 15.232 1.00 18.18 ATOM 957 OH TYR A 185 30.590 13.952 15.232 1.00 18.12 ATOM 957 OH TYR A 185 30.590 13.952 15.232 1.00 18.12 ATOM 958 CD TYR A 185 30.590 13.952 15.232 1.00 18.12 ATOM 950 OF TYR A 185 30.590 13.952 15.232 1.00 18.12 ATOM 950 OF TYR A 185 30.590 13.952 15.232 1.00 18.13 ATOM 950 OF TYR A 185 30.590 13.952 15.232 1.00 18.14 ATOM 950 OF TYR A 185 30.590 13.952 15.232 1.00 18.15 ATOM 950 OF TYR A 185 30.590 13.952 15.232 1.00 18.579 ATOM 960 OF TYR A 185 30.590 13.952 15.232 1.00 18.579 ATOM 960 OF TYR A 186 32.559 18.403 23.094 1.00 16.62 ATOM 960 OF TYR A 186 33.954 16.953 24.019 1.00 14.68 50 ATOM 960 OF TYR A 186 33.954 16.953 24.		ATOM	936	0	ARG	Α	183	30.383	15.333					A
ATOM 938 CA PHE A 184 29.144 13.746 21.722 1.00 18.04 ATOM 939 CB PHE A 184 28.719 11.857 20.098 1.00 22.67 ATOM 940 CG PHE A 184 28.719 11.857 20.098 1.00 22.67 ATOM 941 CD1 PHE A 184 29.317 11.949 18.550 1.00 12.05 ATOM 942 CD2 PHE A 184 29.317 11.949 18.550 1.00 19.97 ATOM 943 CE1 PHE A 184 29.317 11.949 18.550 1.00 19.97 ATOM 944 CE2 PHE A 184 29.915 10.833 18.263 1.00 24.11 30 ATOM 945 CZ PHE A 184 29.915 10.833 18.263 1.00 24.11 30 ATOM 946 C PHE A 184 29.910 9.613 18.928 1.00 22.97 ATOM 947 O PHE A 184 30.403 14.127 20.941 1.00 17.99 ATOM 947 O PHE A 184 31.461 13.531 21.130 1.00 18.89 ATOM 948 N TYR A 185 30.292 15.110 20.056 1.00 15.73 ATOM 949 CA TYR A 185 30.292 15.110 20.056 1.00 15.73 ATOM 950 CB TYR A 185 30.992 16.413 18.111 1.00 17.33 ATOM 951 CG TYR A 185 30.364 15.584 17.015 1.00 19.37 ATOM 953 CE1 TYR A 185 30.364 15.584 17.015 1.00 18.89 ATOM 953 CE1 TYR A 185 30.590 13.895 15.232 1.00 18.12 ATOM 955 CE2 TYR A 185 30.590 13.895 15.232 1.00 18.12 ATOM 955 CE2 TYR A 185 30.590 13.895 15.232 1.00 18.12 ATOM 955 CE2 TYR A 185 30.590 13.895 15.232 1.00 18.18 ATOM 950 CB TYR A 185 30.590 13.895 15.232 1.00 18.18 ATOM 955 CE2 TYR A 185 30.590 13.895 15.232 1.00 18.18 ATOM 956 CZ TYR A 185 30.590 13.895 15.232 1.00 18.18 ATOM 956 CZ TYR A 185 30.590 13.895 15.232 1.00 18.18 ATOM 956 CZ TYR A 185 30.590 13.895 15.232 1.00 18.90 ATOM 958 C TYR A 185 32.544 16.172 20.083 1.00 15.79 ATOM 958 C TYR A 185 32.544 16.172 20.083 1.00 15.79 ATOM 960 N THR A 186 32.559 18.403 23.094 1.00 16.63 ATOM 961 CA THR A 186 32.559 18.403 23.094 1.00 16.63 ATOM 963 CG1 THR A 186 33.565 18.953 24.019 1.00 14.06 ATOM 963 CG1 THR A 186 33.565 18.953 24.019 1.00 14.06 ATOM 966 C THR A 186 33.559 13.595 22.481 1.00 14.79 ATOM 968 CA ALA A 187 33.869 14.196 23.757 1.00 14.06 ATOM 969 CB ALA A 187 33.869 14.196 23.757 1.00 14.06 ATOM 969 CB ALA A 187 33.869 14.196 23.757 1.00 14.06 ATOM 969 CB ALA A 187 33.869 14.196 23.757 1.00 14.01 4.74 ATOM 969 CB ALA A 187 33.869 14.196 23.757 1.00 14.01 4.74 ATOM 969 CB ALA A 187 33.869			937	N	PHE	Α	184	28.520						A
ATOM		ATOM	938	CA	PHE	A	184	29.144						Α
25		ATOM	939	CB	PHE	Α	184	28.158	13.078		1.00	21.05		. A
ATOM 941 CD1 PHE A 184 28.717 10.630 20.754 1.00 22.97 ATOM 942 CD2 PHE A 184 29.317 11.949 18.850 1.00 19.97 ATOM 943 CE1 PHE A 184 29.308 9.510 20.176 1.00 23.53 ATOM 944 CE2 PHE A 184 29.915 10.833 18.263 1.00 24.11 30 ATOM 945 CZ PHE A 184 29.915 10.833 18.263 1.00 22.97 ATOM 946 C PHE A 184 29.910 9.613 18.928 1.00 22.97 ATOM 946 C PHE A 184 31.461 13.531 21.130 1.00 18.89 ATOM 947 O PHE A 184 31.461 13.531 21.130 1.00 18.89 ATOM 949 CA TYR A 185 30.292 15.110 20.056 1.00 15.73 ATOM 949 CA TYR A 185 30.992 16.413 18.111 1.00 17.33 ATOM 951 CG TYR A 185 30.992 16.413 18.111 1.00 17.33 ATOM 951 CG TYR A 185 30.992 16.413 18.111 1.00 17.33 ATOM 952 CD1 TYR A 185 30.364 15.584 17.015 1.00 19.97 ATOM 953 CE1 TYR A 185 30.590 13.952 15.232 1.00 18.12 ATOM 954 CD2 TYR A 185 30.590 13.952 15.232 1.00 18.12 ATOM 955 CE2 TYR A 185 28.976 15.484 16.892 1.00 18.18 ATOM 958 C TYR A 185 29.211 13.861 15.133 1.00 18.41 ATOM 958 C TYR A 185 32.544 16.172 20.083 1.00 15.79 ATOM 958 C TYR A 185 32.544 16.172 20.083 1.00 15.69 ATOM 960 N THR A 186 32.559 18.403 23.094 1.00 16.63 ATOM 962 CB THR A 186 32.559 18.403 23.094 1.00 16.63 ATOM 962 CB THR A 186 32.559 18.403 23.094 1.00 16.63 ATOM 962 CB THR A 186 33.184 17.504 21.997 1.00 16.03 ATOM 962 CB THR A 186 33.844 17.504 21.997 1.00 16.03 ATOM 962 CB THR A 186 33.844 17.504 21.997 1.00 16.63 ATOM 963 OG1 THR A 186 33.844 17.504 21.997 1.00 16.63 ATOM 964 CG2 THR A 186 33.844 17.504 21.997 1.00 16.63 ATOM 965 C THR A 186 33.844 17.504 21.997 1.00 16.63 ATOM 966 C THR A 186 33.954 16.375 22.680 1.00 15.59 ATOM 969 CB ALA A 187 33.234 15.333 23.097 1.00 14.68 ATOM 969 CB ALA A 187 33.234 15.333 23.097 1.00 14.68 ATOM 969 CB ALA A 187 33.234 15.333 23.097 1.00 14.64 ATOM 969 CB ALA A 187 33.234 15.335 24.224 1.00 14.79 ATOM 969 CB ALA A 187 33.234 15.335 24.224 1.00 14.71 ATOM 969 CB ALA A 187 33.234 15.350 22.821 1.00 14.41 ATOM 970 C ALA A 187 33.2810 13.195 24.224 1.00 14.01 ATOM 970 C ALA A 187 33.4875 13.509 22.821 1.00 14.01 ATOM 970 C ALA A 188 35.443 12.704 20.615 1.00	25	ATOM	940	CG	PHE	Α	184							A
ATOM 942 CD2 PHE A 184 29.317 11.949 18.850 1.00 19.97 ATOM 943 CE1 PHE A 184 29.308 9.510 20.176 1.00 23.53 ATOM 944 CE2 PHE A 184 29.915 10.833 18.263 1.00 24.11 30 ATOM 945 CZ PHE A 184 29.910 9.613 18.928 1.00 22.97 ATOM 946 C PHE A 184 30.403 14.127 20.941 1.00 17.99 ATOM 947 O PHE A 184 31.461 13.531 21.130 1.00 18.89 ATOM 948 N TYR A 185 30.292 15.110 20.056 1.00 15.73 ATOM 949 CA TYR A 185 30.992 15.110 20.056 1.00 15.73 ATOM 950 CB TYR A 185 30.992 15.110 20.056 1.00 15.73 ATOM 951 CG TYR A 185 30.364 15.584 17.015 1.00 17.93 ATOM 952 CD1 TYR A 185 30.364 15.584 17.015 1.00 16.53 ATOM 953 CE1 TYR A 185 30.590 13.952 15.232 1.00 18.12 ATOM 955 CE2 TYR A 185 30.590 13.952 15.232 1.00 18.12 ATOM 955 CE2 TYR A 185 28.976 15.484 16.892 1.00 18.12 ATOM 956 CZ TYR A 185 28.976 15.484 16.892 1.00 18.12 ATOM 957 CH TYR A 185 28.398 14.623 15.956 1.00 18.90 ATOM 958 C TYR A 185 28.398 14.623 15.956 1.00 18.90 ATOM 958 C TYR A 185 28.398 14.623 15.956 1.00 18.90 ATOM 958 C TYR A 185 28.398 14.623 15.956 1.00 18.90 ATOM 958 C TYR A 185 28.398 14.623 15.956 1.00 18.90 ATOM 958 C TYR A 185 32.544 16.172 20.083 1.00 15.79 ATOM 959 O TYR A 185 32.544 16.172 20.083 1.00 15.79 ATOM 959 O TYR A 185 33.720 16.015 19.766 1.00 17.69 ATOM 960 N THR A 186 32.559 18.403 23.094 1.00 16.62 ATOM 961 CA THR A 186 32.559 18.403 23.094 1.00 16.62 ATOM 962 CB THR A 186 33.656 18.953 24.019 1.00 16.650 ATOM 962 CB THR A 186 33.656 18.953 24.019 1.00 16.559 ATOM 966 CC THR A 186 33.656 18.953 24.019 1.00 14.68 ATOM 967 N ALA A 187 33.869 14.196 23.757 1.00 14.74 ATOM 969 CB ALA A 187 33.869 14.196 23.757 1.00 14.74 ATOM 969 CB ALA A 187 33.869 14.196 23.757 1.00 14.06 ATOM 969 CB ALA A 187 33.869 14.196 23.757 1.00 14.01 ATOM 969 CB ALA A 187 33.869 14.196 23.757 1.00 14.01 ATOM 969 CB ALA A 187 33.869 14.196 23.757 1.00 14.01 ATOM 969 CB ALA A 187 33.869 14.196 23.757 1.00 14.01 ATOM 969 CB ALA A 187 33.869 14.196 23.757 1.00 14.01 ATOM 969 CB ALA A 187 33.869 14.196 23.757 1.00 14.01 ATOM 969 CB ALA A 187 33.869 14.196 23.757 1.00 14		•	941	CD1				28.717						A
ATOM 943 CE1 PHE A 184 29.308 9.510 20.176 1.00 23.53 ATOM 944 CE2 PHE A 184 29.915 10.833 18.263 1.00 24.11 30 ATOM 945 CZ PHE A 184 29.910 9.613 18.928 1.00 22.97 ATOM 946 C PHE A 184 30.403 14.127 20.941 1.00 17.99 ATOM 947 O PHE A 184 31.461 13.531 21.130 1.00 18.89 ATOM 948 N TYR A 185 30.292 15.110 20.056 1.00 15.73 ATOM 949 CA TYR A 185 30.992 16.413 18.111 1.00 17.33 ATOM 950 CB TYR A 185 30.992 16.413 18.111 1.00 17.33 ATOM 951 CG TYR A 185 30.364 15.584 17.015 1.00 19.37 ATOM 953 CE1 TYR A 185 31.159 14.809 16.168 1.00 16.37 ATOM 953 CE1 TYR A 185 31.159 14.809 16.168 1.00 18.12 ATOM 955 CE2 TYR A 185 28.976 15.484 16.892 1.00 18.18 ATOM 955 CE2 TYR A 185 28.976 15.484 16.892 1.00 18.18 ATOM 955 CE2 TYR A 185 28.976 15.484 16.892 1.00 18.18 ATOM 957 OH TYR A 185 29.211 13.861 15.133 1.00 18.41 ATOM 957 OH TYR A 185 32.544 16.172 20.083 1.00 15.79 ATOM 959 C TYR A 185 33.720 16.015 19.766 1.00 17.69 ATOM 950 CB TYR A 185 33.720 16.015 19.766 1.00 17.69 ATOM 961 CA THR A 186 33.184 17.504 21.997 1.00 16.03 ATOM 963 OG1 THR A 186 32.559 18.403 23.094 1.00 16.62 ATOM 963 OG1 THR A 186 33.184 17.504 21.997 1.00 16.03 ATOM 963 OG1 THR A 186 33.866 18.953 24.019 1.00 14.79 ATOM 966 C THR A 186 33.866 18.953 24.019 1.00 14.79 ATOM 968 CA THR A 186 33.866 18.953 24.019 1.00 14.79 ATOM 968 CA THR A 186 33.866 18.953 24.019 1.00 14.79 ATOM 968 CA ALA A 187 33.234 15.333 23.097 1.00 14.79 ATOM 968 CA ALA A 187 33.234 15.333 23.097 1.00 14.79 ATOM 969 CB ALA A 187 33.234 15.333 23.097 1.00 14.74 ATOM 969 CB ALA A 187 33.869 14.955 23.757 1.00 14.74 ATOM 969 CB ALA A 187 33.869 14.955 23.757 1.00 14.74 ATOM 969 CB ALA A 187 33.869 14.955 23.257 1.00 14.74 ATOM 969 CB ALA A 187 33.869 14.955 23.257 1.00 14.74 ATOM 969 CB ALA A 187 33.869 14.955 23.257 1.00 14.74 ATOM 969 CB ALA A 187 33.869 14.955 23.257 1.00 14.74 ATOM 969 CB ALA A 187 33.869 14.955 23.257 1.00 14.74 ATOM 969 CB ALA A 187 33.869 14.955 23.257 1.00 14.74 ATOM 969 CB ALA A 187 33.869 14.955 23.257 1.00 14.74 ATOM 969 CB ALA A 187 33.869 14.96 23.757				CD2	PHE	Α	184							Α
ATOM				CE1	PHE	Α	184							Α
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ATOM 962 CB THR A 186 32.559 18.403 23.094 1.00 16.62 ATOM 963 OG1 THR A 186 31.866 19.503 22.481 1.00 14.79 ATOM 964 CG2 THR A 186 33.656 18.953 24.019 1.00 14.68 50 ATOM 965 C THR A 186 33.954 16.375 22.680 1.00 15.59 ATOM 966 O THR A 186 35.176 16.443 22.823 1.00 13.77 ATOM 967 N ALA A 187 33.234 15.333 23.097 1.00 14.06 ATOM 968 CA ALA A 187 33.869 14.196 23.757 1.00 14.74 ATOM 969 CB ALA A 187 32.810 13.195 24.224 1.00 14.32 55 ATOM 970 C ALA A 187 34.875 13.509 22.821 1.00 14.41 ATOM 971 O ALA A 187 35.972 13.136 23.247 1.00 15.61 ATOM 972 N GLU A 188 34.516 13.340 21.549 1.00 14.01 ATOM 973 CA GLU A 188 35.443 12.704 20.615 1.00 13.50														A
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50 ATOM 965 C THR A 186 33.954 16.375 22.680 1.00 15.59 ATOM 966 O THR A 186 35.176 16.443 22.823 1.00 13.77 ATOM 967 N ALA A 187 33.234 15.333 23.097 1.00 14.06 ATOM 968 CA ALA A 187 33.869 14.196 23.757 1.00 14.74 ATOM 969 CB ALA A 187 32.810 13.195 24.224 1.00 14.32 55 ATOM 970 C ALA A 187 34.875 13.509 22.821 1.00 14.41 ATOM 971 O ALA A 187 35.972 13.136 23.247 1.00 15.61 ATOM 972 N GLU A 188 34.516 13.340 21.549 1.00 14.01 ATOM 973 CA GLU A 188 35.443 12.704 20.615 1.00 13.50													•	Α
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55 ATOM 970 C ALA A 187 34.875 13.509 22.821 1.00 14.41 ATOM 971 O ALA A 187 35.972 13.136 23.247 1.00 15.61 ATOM 972 N GLU A 188 34.516 13.340 21.549 1.00 14.01 ATOM 973 CA GLU A 188 35.443 12.704 20.615 1.00 13.50														A
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ATOM 973 CA GLU A 188 35.443 12.704 20.615 1.00 13.50														A
														Α
J:		ATOM	974	·CB				34.782	12.449	19.251				Α

	ATOM	975			A 188	33.62	2 11.454	19.282	1.00 12.71	A
	MOTA	976			A 188	33.46	4 10.685	17.979		A
	ATOM	977		GLU 2		33.68	7 11.275	16.899		A
_	ATOM	978		GLU Z		33.11	0 9.484	18.031	1.00 17.69	A
5	ATOM	979	С	GLU Z	A 188	36.68	2 13.582	20.436	1.00 13.34	A
	MOTA	980	0	GLU Z	188	37.80	3 13.085	20.408	1.00 14.69	A
	MOTA	981	N	ILE A	189	36.48	6 14.893	20.326	1.00 13.52	A
	ATOM	982	CA	ILE A	189	37.62	7 15.787	20.159	1.00 13.35	A
	MOTA	983	CB		189	37.16	9 17.247	19.939	1.00 13.95	A
10	MOTA	984	CG2	ILE A	189	38.38	1 18.165	19.822	1.00 12.47	A
	ATOM	985	CG1	ILE A	189	36.30	2 17.332	18.671	1.00 13.44	A
	ATOM	986	CD1	ILE A	189	35.58	3 18.664	18.491	1.00 14.29	A
	ATOM	987	С	ILE A	189	38.53	15.702	21.394	1.00 14.63	A
	MOTA	988	0	ILE A	189	39.75	3 15.595	21.271	1.00 12.97	A
15	ATOM	989	N	VAL A	190	37.92	7 15.751	22.582	1.00 14.35	A
	ATOM	990	CA	VAL A	190	38.68	15.655	23.832	1.00 13.22	A
	ATOM	991	CB	VAL A	190	37.743	15.690	25.061	1.00 14.28	A
	ATOM	992	CG1	VAL A		38.509	15.267	26.326	1.00 15.08	A
	ATOM	993	CG2	VAL A	190	37.160		25.233	1.00 12.08	A
20	ATOM	994	С	VAL A	190	39.468		23.859	1.00 14.61	A
	ATOM	995	0	VAL A	190	40.634	14.304	24.250	1.00 13.72	A
	ATOM	996	N	SER A	191	38.825		23.432	1.00 15.26	A
	ATOM	997	CA	SER A	191	39.478	11.943	23.421	1.00 16.81	A
	MOTA	998	СВ	SER A	191	38.470	10.857	23.041	1.00 16.14	A
25	MOŢA	999	OG	SER A	191	39.018	•	23.238	1.00 16.94	A
	MOTA	1000	С	SER A	191	40.649		22.441	1.00 16.58	A
	MOTA	1001	0	SER A	191	41.697	11.335	22.713	1.00 13.96	A
	MOTA	1002	N	ALA A	192	40.468	12.586	21.300	1.00 15.26	A
	ATOM	1003	CA	ALA A	192	41.518	12.645	20.292	1.00 14.37	A
30	ATOM	1004	CB	ALA A	192	40.989		19.016	1.00 14.43	A
	MOTA	1005	С	ALA A	192	42.695	13.440	20.845	1.00 16.46	A
	ATOM	1006	0	ALA A	192	43.851		20.697	1.00 17.96	A
	ATOM	1007	N	LEU A	193	42.401	14.563	21.496	1.00 15.02	A
	MOTA	1008	CA	LEU A	193	43.459		22.067	1.00 15.42	A
35	ATOM	1009	CB	LEU A	193	42.884		22.600	1.00 12.88	A
	MOTA	1010	CG	LEU A		42.445		21.525	1.00 15.97	`A
	ATOM	1011	CD1	LEU A	193	41.869		22.190	1.00 13.97	. А
	MOTA	1012	CD2	LEU A	193	43.642	18.088	20.655	1.00 14.58	A
	MOTA	1013	С	LEU A	193	44.211		23.174	1.00 14.49	A
40	MOTA	1014	0	LEU A	193	45.427		23.310	1.00 16.56	A
	ATOM	1015	N	GLU A	194	43.500		23.975	1.00 13.96	A
	MOTA	1016	CA	GLU A	194	44.179		25.032	1.00 14.08	A
	MOTA	1017	CB	GLU A	194	43.190	12.295	25.857	1.00 14.65	A
	MOTA	1018	CG	GLU A	194	43.882	11.301	26.789	1.00 17.09	A
45	ATOM	1019	CD	GLU A	194	42.924	10.592	27.730	1.00 19.59	A
	ATOM	1020	OE1	GLU A	194	41.809		27.295	1.00 19.25	A
	ATOM	1021	OE2	GLU A	194	43.302		28.906	1.00 20.20	A
	ATOM	1022		GLU A		45.208	12.199	24.386	1.00 13.57	A
	ATOM	1023	0	GLU A	194	46.337	12.093	24.847	1.00 14.23	A
50	ATOM	1024	N	TYR A	195	44.822	11.544	23.301	1.00 14.89	A
	ATOM	1025	CA	TYR A	195	45.743	10.642	22.618	1.00 16.58	A
	MOTA	1026	CB	TYR A	195	45.030	9.910	21.488	1.00 17.29	A
	ATOM	1027	CG	TYR A	195	45.956	9.058	20.649	1.00 17.92	A
	ATOM	1028	CD1	TYR A	195	46.347	7.788	21.077	1.00 17.96	A
55	ATOM	1029		TYR A		47.203	6.996	20.304	1.00 19.77	A
	ATOM	1030	CD2	TYR A	195	46.445	9.524	19.428	1.00 16.67	A
	ATOM	1031	CE2	TYR A	195	47.299	8.744	18.650	1.00 18.51	A
	MOTA	1032		TYR A		47.671	7.481	19.094	1.00 20.24	A
	ATOM	1033		TYR A		48.506	6.705	18.325	1.00 21.89	A

	ATOM	1034	С	TYR .	A 195	46.9	17 11.419	22.035	1.00 16.98	А
	ATOM	1035	0	TYR .	A 195	48.0				
	ATOM	1036	N	LEU .	A 196	46.5			1.00 16.30	
	ATOM	1037	CA		A 196				1.00 18.15	A
5	ATOM	1038	CB	LEU .	A 196				1.00 18.59	
	ATOM	1039	CG		A 196				1.00 22.51	A
	ATOM	1040		LEU					1.00 20.94	A
	ATOM	1041		LEU					1.00 20.94	A
	ATOM	1042	C		A 196	-		21.763	1.00 22.98	
10	ATOM	1043	Ö		A 196			21.649	1.00 17.73	A A
	ATOM	1044	N		1 197			22.792	1.00 18.33	A
	ATOM	1045	CA		1 197	48.9		23.842	1.00 17.12	
	ATOM	1046	CB		1 197			24.817	1.00 15.47	A A
	ATOM	1047	CG		1 197			24.231	1.00 19.15	
15	ATOM	1048		HIS A	-			23.038	1:00 19:15	A
	ATOM	1049		HIS A		46.7		24.897		A
	ATOM	1050		HIS A		46.4		24.097	1.00 17.47	A
	ATOM	1051		HIS A		47.1			1.00 19.74	A
	ATOM	1052	C	HIS A		49.6		23.007	1.00 15.69	A
20	ATOM	1052	Ö	HIS A				24.572	1.00 19.40	A
20	ATOM	1053		GLY A		50.8		25.021	1.00 19.42	A
	ATOM	1054	N CA	GLY A		49.1		24.679	1.00 18.59	A
	ATOM	1056	C			49.7		25.339	1.00 19.60	A
	ATOM	1050		GLY F		51.0		24.612	1.00 21.86	. A
25			0	LYS A		51.9		25.186	1.00 23.09	A
23	MOTA	1058	N			51.1	•	23.341	1.00 22.81	A.
	ATOM ATOM	1059 1060	CA	LYS A		52.3		22.549	1.00 24.43	A
			CB	LYS A		51.9		21.154	1.00 26.00	A
	MOTA	1061	CG	LYS A		51.3		21.133	1.00 30.98	A
30	ATOM ATOM	1062	CD	LYS A		512		19.708	100 36.85	A
30	ATOM	1063	CE	LYS A		50.8		19.682	1.00 40.37	A
	ATOM	1064 1065	NZ C	LYS F		51.6 53.2		20.581	1.00 43.48	A
	ATOM							22.414	1.00 23.88	A
	ATOM	1066	0	LYS F		54.1		21.568	1.00 24.97	Ą
35	ATOM	1067 1068	N CA	GLY A		52.9		23.243	1.00 24.00	A
33	ATOM	1069	CA	GLY A		53.7		23.203	1.00 22.12	A
	ATOM	1009		GLY A		53.69 54.63		21.907	1.00 22.14 1.00 22.41	A
	ATOM	1070	O N	ILE A		52.4		21.439		A
		1071						21.320	1.00 20.00	A
40	ATOM ATOM	1072	CA CB	ILE A		52.25 51.78		20.080	1.00 18.93	A
40	ATOM	1073		ILE A		51.7		18.955 17.716	1.00 19.70 1.00 20.12	A A
	ATOM	1074		ILE A		52.88		18.636	1.00 20.12	
	ATOM	1075		ILE A		52.40		17.745	1.00 20.03	A A
	ATOM	1070	CDI	ILE A		51.19		20.270	1.00 22.75	
45										A
73	ATOM ATOM	1078	0	ILE A		50.12		20.817	1.00 20.08	A
•	ATOM	1079 1080	N CA	ILE A		51.50		19.815 19.891	1.00 19.94	A
				ILE A		50.60			1.00 20.45	A
	ATOM ATOM	1081 1082	CB			51.35		20.356	1.00 22.21	A
50				ILE A		50.38		20.470	1.00 22.67	A
50	ATOM	1083 1084		ILE A		52.03		21.700	1.00 24.19	A
	ATOM ATOM		CD1 C	ILE A		52.91		22.169	1.00 25.39	A
		1085				50.10		18.464	1.00 20.71	· A
	ATOM	1086	O N	ILE A		50.91		17.538	1.00 19.48	A n
55	ATOM	1087	N			48.79		18.270	1.00 18.65	A
<i>J J</i>	ATOM	1088	CA	HIS A		48.28		16.919	1.00 18.02	A
	ATOM	1089	CB	HIS A		46.77		16.874	1.00 16.31	A
	ATOM	1090	CG	HIS A		46.19		15.495	1.00 18.36	A
	ATOM ATOM	1091 1092		HIS A		46.04		14.655	1.00 16.42	A
	AIOM	1032	MDT	пто А	203	45.75	9 19.026	14.806	1.00 19.50	A

								•			
	MOTA	1093		1 HIS			45.359	19.389	13.600	1.00 17.64	A
	MOTA	1094	NE	2 HIS .	A 203		45.522	20.694	13.483	1.00 20.87	 A
	ATOM	1095	С		A 203		48.589	21.738	16.405	1.00 18.92	A
_	ATOM	1096	0		A 203		49.073	21.906	15.282	1.00 16.21	A
5	MOTA	1097	N		A 204		48.301	22.744	17.232	1.00 18.60	A
	ATOM	1098	CA	ARG I	A 204		48.552	24.157	16.914	1.00 19.81	A
	ATOM	1099	СВ	ARG A	A 204		49.998	24.365	16.458	1.00 21.61	A
	ATOM	1100	CG	ARG I	A 204		51.024	24.137	17.550	1.00 23.82	A
	MOTA	1101	CD	ARG A	A 204		52.323	24.870	17.252	1.00 27.62	A
10	ATOM	1102	NE	ARG A	A 204		52.932	24.449	15.994	1.00 29.43	A
	ATOM	1103	CZ	ARG A	A 204		54.125	24.861	15.572	1.00 33.10	A
	ATOM	1104	NH				54.835	25.706	16.311	1.00 32.12	A
	ATOM	1105	NH2	2 ARG A			54.614	24.426	14.418	1.00 30.25	A
	ATOM	1106	С	ARG A			47.624	24.830	15.905	1.00 20.03	A
15	ATOM	1,107	0	ARG A			47.711	26.038	15.698	1.00 20.88	A
	ATOM	1108	N	ASP A			46.755	24.071	15.255	1.00 18.96	A
	ATOM	1109	CA	ASP A			45.828	24.692	14.325	1.00 17.90	A
	ATOM	1110	CB	ASP A			46.418	24.741	12.914	1.00 18.95	A
	MOTA	1111	CG	ASP F			45.655	25.688	12.008	1.00 20.36	A
20	ATOM	1112		ASP A			44.939	26.560	12.545	1.00 20.35	A
	ATOM	1113		ASP A			45.772	25.573	10.771	1.00 22.49	A
	ATOM	1114	С	ASP A			44.500	23.956	14.328	1.00 19.60	A
	MOTA	1115	0	ASP A			43.876	23.751	13.287	1.00 21.53	A
	ATOM	1116	N	LEU A			44.063	23.569	15.521	1.00 18.53	A
25	ATOM	1117	CA	LEU A			42.813	22.851	15.667	1.00 19.18	A
	ATOM	1118	CB	LEU A			42.693	22.295	17.087	1.00 18.94	A
	ATOM	1119	CG	LEU A			41.511	21.358	17.346	1.00 23.10	Ā
	ATOM	1120		LEU A			41.615	20.142	16.436	1.00 23.10	A
	ATOM	1121		LEU A			41.504	20.933	18.808	1.00 22.97	A
30	ATOM	1122	С	LEU A			41.639	23.772	15.361	1.00 19.05	A
	ATOM	1123	0	LEU A			41.556	24.880	15.886	1.00 19.25	A
	ATOM	1124	N	LYS A			40.740	23.307	14.500	1.00 17.54	A
	ATOM	1125	CA	LYS A	207		39.564	24.081	14.110	1.00 18.60	A
	ATOM	1126	CB	LYS A	207		39.980	25.248	. 13.196	1.00 18.98	A
35	ATOM	1127	CG	LYS A	207		40.786	24.817	11.982	1.00 18.20	A
	ATOM	1128	CD	LYS A	207		41.246	26.000	11.139	1.00 21.42	Α
	MOTA	1129	CE	LYS A	207		42.223	25.537	10.062	1.00 23.21	Α
	ATOM	1130	· NZ	LYS A	207		42.561	26.604	9.084	1.00 29.61	Α
	ATOM	1131	С	LYS A	207		38.566	23.181	13.388	1.00 18.18	A
40	MOTA	1132	0	LYS A	207		38.921	22.100	12.915	1.00 18.11	A
	MOTA	1133	N	PRO A	208		37.298	23.614	13.293	1.00 20.26	. A
	ATOM	1134	CD	PRO A	208.		36.713	24.833	13.882	1.00 18.79	A
	ATOM	1135	CA	PRO A			36.272	22.814	12.616	1.00 19.67	A
	MOTA	1136	CB	PRO A	208		35.063	23.742	12.608	1.00 19.45	A
45	MOTA	1137	CG	PRO A	208		35.231	24.509	13.891	1.00 21.81	A
	ATOM	1138	С	PRO A	208		36.674	22,372	11.209	1.00 21.04	A
	ATOM	1139	0	PRO A	208		36.264	21.307	10.751	1.00 21.19	A
	ATOM	1140	N	GLU A	209		37.474	23.188	10.528	1.00 21.69	A
	MOTA	1141	CA	GLU A	209		37.928	22.872	9.170	1.00 22.64	A
50	ATOM	1142	CB	GLU A	209		38.644	24.084	8.558	1.00 23.65	A
	ATOM	1143	CG	GLU A	209		39.253	23.825	7.185	1.00 27.24	A
	ATOM	1144	CD	GLU A	209		40.155	24.958	6.716	1.00 29.40	A
	ATOM	1145	OE1	GLU A	209		39.660	26.094	6.553	1.00 29.68	A
	ATOM	1146	OE2	GLU A	209		41.363	24.711	6.511	1.00 30.07	Α
55 .	MOTA	1147	С	GLU A			38.879	21.668	9.159	1.00 22.28	A
	ATOM	1148	0	GLU A			38.955	20.933	8.170	1.00 21.36	A
	MOTA	1149	N	ASN A	210		39.600	21.490	10.263	1.00 19.90	A
	MOTA	1150	CA	ASN A	210		40.574	20.412	10.436	1.00 19.44	A
	ATOM	1151	CB	ASN A	210		41.744	20.912	11.287	1.00 20.07	A
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	ATOM	1152		. 42.746	21.698	10.479	1.00 25.77	. А
	MOTA	1153	OD1 ASN A 210	43.571	22.427	11.029	1.00 26.73	Α
	ATOM	1154	ND2 ASN A 210	42.687	21.548	9.158	1.00 25.15	A
_	MOTA	1155	C ASN A 210	40.005	19.151	11.078	1.00 18.63	Α
5	ATOM	1156	O ASN A 210	40.712	18.154	11.234	1.00 18.29	Α
	MOTA	1157	N ILE A 211	38.739	19.202	11.469	1.00 16.31	A
	ATOM	1158	CA ILE A 211	38.090	18.058	12.085	1.00 15.49	A
	ATOM	1159	CB ILE A 211	37.336	18.488	13.354	1.00 15.40	A
	ATOM	1160	CG2 ILE A 211	36.582	17.311	13.950	1.00 14.59	A
10	ATOM	1161	CG1 ILE A 211	38.342	19.046	14.365	1.00 15.91	A
	ATOM	1162	CD1 ILE A 211	37.720	19.669	15.590	1.00 15.98	A
	ATOM	1163	C ILE A 211	37.131	.17.485	11.059	1.00 17.26	A
	ATOM	1164	O ILE A 211	35.995	17.947	10.926	1.00 18.16	A
	MOTA	1165	N LEU A 212	37.599	16.486	10.317	1.00 15.97	A
15	ATOM	1166	CA LEU A 212	36.784	15.875	9.274	1.00 17.08	A
	MOTA	1167	CB LEU A 212	37.685	15.249	8.202	1.00 17.78	A
	ATOM	1168	CG LEU A 212	38.785	16.157	7.640	1.00 17.70	A
	ATOM	1169	CD1 LEU A 212	39.476	15.450	6.485	1.00 22.09	A
	ATOM	1170	CD2 LEU A 212	38.188	17.482	7.166	1.00 19.91	A
20	ATOM		C LEU A 212	35.843	14.825	9.837	1.00 18.35	A
	ATOM	1172	O LEU A 212	35.957	14.433	11.002	1.00 10.33	A
	ATOM	1173	N LEU A 213	34.915	14.368	9.000	1.00 17.84	A
	ATOM	1174	CA LEU A 213		13.362	9.403	1.00 17.84	A
	ATOM	1175	CB LEU A 213	32.556	14.004	9.487	1.00 19.94	A
25	MOTA	1176	CG LEU A 213	32.396	15.059	10.583	1.00 20.34	A
	ATOM	1177	CD1 LEU A 213	.31,124	15.837	10.367	1.00 20.31	A
	ATOM	1178	CD2 LEU A 213	32.379	14.378	11.940	1.00 22.73	A
	ATOM	1179	C LEU A 213	33.914	12.187	8.426	1.00 20.98	A
	MOTA	1180	O LEU A 213	33.743	12.379	7.218	1.00 20.50	A
30	ATOM	1181	N ASN A 214	34.088	10.970	8.935	1.00 20.44	A
	ATOM	1182	CA ASN A 214	34.055	9.814	8.049	1.00 23.77	A
	ATOM	1183	CB ASN A 214	34.745	8.596	8.674	1.00 25.30	· A
	ATOM	1184	CG ASN A 214	34.077	8.127	9.948	1.00 32.04	A
	ATOM	1185	OD1 ASN A 214	32.908	8.422	10.206	1.00 34.43	A
35	ATOM	1186	ND2 ASN A 214	34.818	7.369	10.752	1.00 33.85	A
	ATOM	1187	C ASN A 214	32.618	9.466	7.693	1.00 24.07	Α
	ATOM	1188	O ASN A 214	31.672	10.113	8.150	1.00 19.94	A
	ATOM	1189	N GLU A 215	32.459	8.433	6.879	1.00 25.77	Α
	MOTA	1190	CA GLU A 215	31.138	8.003	6.445	1.00 28.69	A
40	ATOM	1191	CB GLU A 215	31.275	6.796	5.513	1.00 31.98	А
	ATOM	1192	CG GLU A 215	29.970	6.334	4.896	1.00 40.22	·A
	ATOM	1193	CD GLU A 215	30.182	5.312	3.795	1.00 44.27	A
	ATOM	1194	OE1 GLU A 215	30.817	4.268	4.065	1.00 46.46	A
	MOTA	1195	OE2 GLU A 215	29.716	5.556	2.660	1.00 46.13	A
45	ATOM	1196	C GLU A 215	30.188	7.673	7.601	1.00 28.41	A
	MOTA	1197	O GLU A 215	28.971	7.769	7.447	1.00 28.52	A
	MOTA	1198	N ASP A 216	30.737	7.287	8.752	1.00 26.77	A
	ATOM	1199	CA ASP A 216	29.914	6.953	9.917	1.00 27.28	A
	MOTA	1200	CB ASP A 216	30.538	5.795	10.696	1.00 31.27	A
50	ATOM	1201	CG ASP A 216	30.390	4.466	9.979	1.00 37.61	A
	ATOM	1202	OD1 ASP A 216	29.274	4.170	9.499	1.00 39.45	A
	ATOM	1203	OD2 ASP A 216	31.382	3.710	9.902	1.00 41.84	Α
	ATOM	1204	C ASP A 216	29.697	8.135	10.862	1.00 26.37	A
	MOTA	1205	O ASP A 216	29.136	7.984	11.950	1.00 25.73	A
55	ATOM	1206	N MET A 217	30.156	9.306	10.441	1.00 23.02	A
	ATOM	1207	CA MET A 217	30.015	10.527	11.218	1.00 21.83	A
	MOTA	1208	CB MET A 217	28.537	10.789	11.517	1.00 23.24	A
	ATOM	1209	CG MET A 217	27.742	11.186	10.274	1.00 22.98	A
	ATOM	1210	SD MET A 217	28.464	12.616	9.430	1.00 27.57	Α

	ATOM	1211	CE	MET	Α	217	27.679	13.974	10.332	1.00 26.68	A
	ATOM	1212	С			217	30.844	10.618	•		
									12.502	1.00 21.51	
	ATOM	1213	0	MET	A	217	30.474	11.323	13.440	1.00 18.62	A
	ATOM	1214	N	HIS	Α	218	31.957	9.892	12.544	1.00 20.10	A
5	ATOM	1215	CA	HTS	A	218	32.873	9.964	13.678	1.00 19.86	
-											A
	ATOM	1216	CB			218	33.482	8.594	13.977	1.00 20.21	A
	ATOM	1217	CG	HIS	Α	218	32.551	7.667	14.698	1.00 22.40	A
	ATOM	1218	CD2	HIS	Α	218	31.910	6.547	14.287	1.00 21.27	A
	ATOM	1219		HIS			32.177	7.863	16.011		
10										1.00 19.59	
10	MOTA	1220		HIS			31.348	6.902	16.379	1.00 21.88	Α
	ATOM	1221	NE2	HIS	Α	218	31.168	6.091	15.351	1.00 22.08	A
	ATOM	1222	С	HIS	Α	218	33.947	10.921	13.172	1.00 19.10	A
	ATOM	1223	Ó			218	34.170	11.004	11.965	1.00 20.31	
											A
	MOTA	1224	N			219	34.617	11.638	14.067	1.00 17.21	A.
15	MOTA	1225	CA	ILE	Α	219	35.628	12.586	13.618	1.00 15.26	Α
	ATOM	1226	CB	ILE	Α	219	35.987	13.614	14.716	1.00 15.38	A
	ATOM	1227		ILE			34.722	14.305	15.221		
										1.00 14.58	A
	MOTA	1228		ILE			36.734	12.919	15.864	1.00 14.46	A
	ATOM	1229	CD1	ILE	Α	219	37.279	13.885	16.911	1.00 13.74	A
20	MOTA	1230	С	ILÈ	Α	219	36.929	11.944	13.161	1.00 16.21	A
	ATOM	1231	Ō			219	37.238	10.799	13.500		
										1.00 15.88	A
	MOTA	1232	N	GLN	А	220	37.677	12.711	12.378	1.00 15.62	A
	MOTA	1233	CA	GLN	Α	220	38.980	12.316	11.876	1.00 17.84	A
	MOTA	1234	CB	GLN	Α	220	38.872	11.595	10.525	1.00 20.00	Α
25	ATOM	1235	CG	GLN			38.463	10.129	10.659	1.00 26.97	A
23											
	ATOM	1236	CD	GLN			38.648	9.343	9.372	1.00 29.95	A
	ATOM	1237	OE1	GLN	A.	220	37.968	9.590	8.373	1.00 33.12	Α
	ATOM	1238	NE2	GLN	Α	220	39.578	8.393	9.389	1.00 30.47	A
	ATOM	1239	С	GLN	20	220	39.757	13.610	11.735	1.00 17.00	A
20											
30	ATOM	1240	0	GLN			39.609	14.339	10.751	1.00 18.27	A
	ATOM	1241	N	ILE	A	221	40.566	13.906	12.746	1.00 14.34	A
	ATOM	1242	CA	ILE	Α	221	41.361	15.120	12.753	1.00 14.46	A
	ATOM	1243	CB	ILE			41.867	15.416	14.175	1.00 12.30	. A
	MOTA	1244		ILE			42.764	16.656	14.167	1.00 14.78	A
35	MOTA	1245	CGl	ILE	Α.	221	40.660	15.613	15.102	1.00 13.92	A
	ATOM	1246	CD1	ILE	Α	221	41.003	15.901	16.543	1.00 15.06	Α
	ATOM	1247	С	ILE	А	221	42.536	14.996	11.783	1.00 15.44	A
	ATOM	.1248	ō	ILE			43.106	13.915	11.613	1.00 13.93	A
	MOTA	1249	N	THR			42.877	16.101	11.127	1.00 15.36	A
40	ATOM	1250	CA	THR	A	222	43.980	16.098	10.174	1.00 17.52	Α
	ATOM	1251	CB	THR	Α	222	43.470	15.836	8.750	1.00 19.92	A
	ATOM	1252		THR			44.587	15.637	7.875	1.00 18.78	A
	MOŢA	1253		THR			42.630	17.018	8.257	1.00 18.16	A
	ATOM	1254	С	THR			44.735	17.428	10.192	1.00 19.60	A
45	ATOM	1255	0	THR	Α	222	44.509	18.257	11.084	1.00 18.59	. A
	ATOM	1256	N	ASP			45.630	17.610	9.216	1.00 18.69	А
		1257		ASP				18.825	9.069	1.00 20.12	A
	ATOM		CA				46.440				
	ATOM	1258	CB	ASP	·A	223	45.532	20.065	9.108	1.00 23.51	A
	ATOM	1259	CG	ASP	Α	223	46.248	21.335	8.670	1.00 27.09	A
50	ATOM-	1260	001	ASP	Д	223	47.283	21.227	7.975	1.00 26.28	A
		1261		ASP			45.765			1.00 26.15	A
	ATOM							22.438	9.009		
	ATOM	1262	С	ASP			47.516	18.913	10.150	1.00 21.73	A
	ATOM	1263	0	ASP	Α	223	47.439	19.751	11.055	1.00 22.76	A
	ATOM	1264	N	PHE			48.535	18.063	10.027	1.00 20.75	A
55	ATOM	1265		PHE			49.611	17.988	11.009	1.00 20.11	A
JJ											
	ATOM	1266	CB	PHE			49.805	16.527	11.424	1.00 20.62	A
	ATOM	1267	CG	PHE	A	224	48.682	15.991	12.263	1.00 21.41	· A
	ATOM	1268	CD1	PHE	Α	224	48.598	16.312	13.614	1.00 23.05	A
	ATOM	1269		PHE			47.681	15.212	11.693	1.00 22.27	A
	PILON	1209	UD2		4.2	7	27.001	-5.212			**

	ATOM	1270	CE	1 PHE	A 224		47.528	15.868	14.389	1 00	23.30	А
	ATOM	1271	CE		A 224		46.606	14.763	12.457		21.11	
	ATOM	1272	CZ		A 224		46.530	15.093	13.807			
	ATOM	1273	C		A 224						22.02	A
5							50.957	18.583	10.619		20.45	A
3	ATOM	1274	0		A 224		51.905	18.547	11.407		20.73	Α
	ATOM	1275	N		A 225		51.049	19.125	9.412	1.00	22.02	A
	ATOM	1276	CA	GLY	A 225		52.301	19.713	8.981	1.00	22.66	A
	MOTA	1277	С	GLY	A 225		52.742	20.822	9.920	1.00	24.99	A
	ATOM	1278	0	GLY	A 225	•	53.939	21.041	10.122		24.52	A
10	MOTA	1279	N		A 226		51.779	21.524	10.508		23.50	· A
	MOTA	1280	CA		A 226		52.106	22.613	11.416		25.16	A
	ATOM	1281	CB		A 226		51.199	23.829	11.160		24.76	A
	ATOM	1282	OG		A 226	2	49.831	23.410				
									11.113		22.68	A
1.5	ATOM	1283		2 THR			51.571	24.490	9.834		25.00	A
15	ATOM	1284	С		A 226	_	52.046	22.233	12.894		25.79	A
	ATOM	1285	0		A 226		52.019	23.100	13.768		24.54	A
	MOTA	1286	N		A 227		52.037	20.935	13.173	1.00	24.97	A
	MOTA	1287	CA	ALA	A 227		52.004	20.475	14.550	1.00	25.49	A
	ATOM	1288	CB	ALA	A 227		51.659	18.993	14.607	1.00	22.85	A
20	ATOM	1289	С	ALA	A 227		53.384	20.715	15.149		27.70	A
	MOTA	1290	0		A 227		54.331	21.047	14.435		26.60	A
	ATOM	1291	N		A 228		53.491	20.558	16.461		28.53	A
	ATOM	1292	CA		A 228		54.760	20.745	17.149		32.12	A
	ATOM	1293										
0.5			CB		A 228		54.699		18.054		33.81	A
25	MOTA	1294	CG		A 228		56.007	22.294	18.765		41.23	· A
	ATOM	1295	CD		A 228		57.082	22.725	17.768		47.57	A
	MOTA	1296	CE		A 228		58.401	23.056	18.462		49.82	A
	MOTA	1297	NZ	LYS .	A 228		59.459	23.425	17.480	1.00	51.49	A
	ATOM	1298	С	LYS .	A 228	•	55.019	19.504	17.985	1.00	33.25	A
30	MOTA	1299	0	LYS .	A 228		54.190	19.129	18.815	1.00	33.70	A
	ATOM	1300	N	VAL .	A 229		56.159	18.860	17.756	1.00	33.64	A
	MOTA	1301	CA		A 229		56.516	17.661	18.501		34.66	A
	ATOM	1302	СВ		A 229		57.248	16.646	17.609		33.50	A
	ATOM	1303		VAL			57.619	15.419	18.415		32.34	A
35	ATOM	1304		VAL			56.370	16.264	16.436		34.25	A
33												
	ATOM	1305	C		A 229		57.420	18.035	19.668		37.57	A
	ATOM	1306	0		A 229		58.581	18.392	19.474	••	35.91	A
	ATOM	1307	N		A 230		56.877	17.948	20.878		40.57	Α
	ATOM	1308	CA		A 230	-	57.615	18.289	22.088		46.10	A
40	ATOM	1309	CB	LEU A	A 230		56.654	18.417	23.270	1.00	44.71	A
	ATOM	1310	CG	LEU I	A 230		55.627	19.545	23.207	1.00	44.50	Α
	ATOM	1311	CD1	LEU Z	A 230		54.673	19.430	24.383	1.00	44.39	A
	ATOM	1312	CD2	LEU Z	A 230		56.340	20.885	23.214	1.00	44.81	А
	ATOM	1313	С	LEU A	A 230		58.695	17.279	22.440	1.00	50.42	A
45	ATOM	1314	0	LEU Z	A 230		58.603	16.104	22.089	1.00	51.64	A
	ATOM	1315	N		A 231		59.717	17.756	23.145		55.81	A
	ATOM	1316	CA		A 231		60.824	16.914	23.583		61.14	A
	ATOM	1317	CB		A 231		62.077	17.200			61.27	
									22.750			A
50	ATOM	1318	OG		A 231		62.444	18.568	22.823		62.85	A
50	ATOM	1319	С		A 231		61.124	17.126	25.071		64.65	Α
	ATOM	1320	0		A 231		61.392	16.164	25.794		65.70	A
	ATOM	1321	N		A 232		61.081	18.387	25.549		67.54	A
	ATOM	1322	CD	PRO A	A 232		60.854	19.651	24.823	1.00	68.60	A
	ATOM	1323	CA	PRO A	A 232		61.358	18.655	26.966	1.00	68.74	· A
55	ATOM	1324	CB		A 232		61.109	20.158	27.086	1.00	68.83	A
	ATOM	1325	CG		A 232		61.505	20.666	25.737		68.96	A
	ATOM	1326	C		A 232		60.460	17.846	27.899		69.17	A
	ATOM	1327	ō		A 232		59.335	17.494	27.541		69.94	A
	ATOM	1328	N	ALA A			57.424	23.198	27.637		80.06	A
	111013	1020	••	TIME F	- 23,		57.323	~~.190	21.001	1.00	20.00	47

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	MOŢA	1329) C2	A ALA A 237	56.783	23,047	26.335	1.00 79.29	7
	ATOM	1330) CE	•	55.275	•			A
	ATOM	1331	С	ALA A 237	57.092				A
	ATOM	1332		ALA A 237	56.250				P
5	ATOM	1333							A
•	ATOM	1334			58.297				A
					58.683				A
	ATOM	1335			60.186		23.728	1.00 78.50	A
	MOTA	1336		ALA A 238	57.920	25.327	22.673		A
	MOTA	1337		ALA A 238	57.243	24.341	22.375		A
10	ATOM	1338	N	ALA A 239	58.027				A
	ATOM	1339	CA	ALA A 239	57.338				
	ATOM	1340	CB	ALA A 239	55.849				A
	ATOM	1341	С	ALA A 239	57.766			1.00 76.61	A
	MOTA	1342	Ō	ALA A 239	58.955			1.00 75.38	A
15	ATOM	1343	N	ASN A 240				1.00 75.89	A
	ATOM	1344			56.781			1.00 73.95	A
			CA		56.967		18.389	1.00 71.07	A
	ATOM	1345	CB		58.151	30.400	18.874	1.00 71.47	Α
	ATOM	1346	CG		59.459	30.055	18.174	1.00 72.06	A
	ATOM	1347	OD	1 ASN A 240	59.575	30.149	16.943	1.00 72.03	A
20	ATOM	1348		2 ASN A 240	60.470	29.665	18.964	1.00 71.91	A
	MOTA	1349	C	ASN A 240	57.188	29.178	16.928	1.00 69.41	A
	MOTA	1350	0	ASN A 240	57.480	28.024	16.624	1.00 70.09	A
	ATOM	1351	N	ALA A 241	57.055	30.165	16.038	1.00 66.62	
	ATOM	1352	CA		57.246	30.013	14.585	1.00 63.94	A
25	ATOM	1353	С	ALA A 241	55.952	30.080			A
	ATOM	1354	Ō	ALA A 241	55.840	30.880	13.772	1.00 60.63	Α
	`ATOM	1355	СB	ALA A 241	57.979		12.845	1.00 61.29	Α
	ATOM	1356	N	PHE A 242		28.704	14.246	1.00 65.23	A
	ATOM	1357	CA	PHE A 242	54.984	29.236	14.113	1.00 56.72	Α
30	ATOM	1358	CB		53.712	29.196	13.394	1.00 52.53	Α
20	ATOM	1359		PHÈ A 242	53.419	27.767	12.923	1.00 49.14	Α
	ATOM		CG	PHE A 242	52.040	27.590	12.354	1.00 47.38	Α
		1360		PHE A 242	51.731	28.067	11.085	1.00 47.69	A
	ATOM	1361		PHE A 242	51.038	26.975	13.102	1.00 45.45	Α
25	ATOM	1362		PHE A 242	50.445	27.937	10.565	1.00 46.75	A
35	ATOM	1363		PHE A 242	49.751	26.840	12.594	1.00 45.41	A
	MOTA	1364	CZ	PHE A 242	49.453	27.323	11.322	1.00 46.55	· А
	ATOM .	1365	С	PHE A 242	52.534	29.688	14.229	1.00 50.08	A
	ATOM	1366	0	PHE A 242	52.502	29.505	15.444	1.00 49.86	A
	MOTA	1367	N	VAL A 243	51.566	30.305	13.557	1.00 47.67	A
40	ATOM	1368	CA	VAL A 243	50.355	30.809	14.200	1.00 46.21	
	ATOM	1369	CB	VAL A 243	50.340	32.352	14.258	1.00 47.36	A
	ATOM	1370	CG1	VAL A 243	49.012	32.844	14.825		A
	ATOM	1371		VAL A 243	51.497	32.842		1.00 47.54	A
	ATOM	1372	C	VAL A 243	49.150		15.109	1.00 48.50	A
45	ATOM	1373				30.342	13.389	1.00 44.12	A
	ATOM	1374				30.765	12.247	1.00 44.46	Α
	ATOM	1375	N	GLY A 244	48.348	29.467	13.985	1.00 40.48	Α
	ATOM		CA	GLY A 244	47.176	28.941	13.306	1.00 37.65	A
		1376	С	GLY A 244	46.101	29.960	12.964	1.00 35.39	A
50	ATOM	1377	0	GLY A 244	46.313	31.168	13.065	1.00 35.92	A
50	MOTA	1378	N	THR A 245	44.936	29.463	12.560	1.00 33.30	A
	MOTA	1379	CA	THR A 245	43.813	30.312	12.184	1.00 30.20	A
	MOTA	1380	CB	THR A 245	42.593	29.450	11.829	1.00 32.00	A
	ATOM	1381	OG1	THR A 245	42.952	28.573	10.755	1.00 32.81	Ā
	ATOM	1382	CG2	THR A 245	41.419	30.319	11.390	1.00 32.81	
55	ATOM	1383	С	THR A 245	43.476	31.296	13.296	1.00 28.34	A
	ATOM	1384	ō	THR A 245	43.212	30.907			A
	ATOM	1385	N	ALA A 246	43.486		14.434	1.00 25.46	A
	ATOM	1386	CA	ALA A 246		32.576	12.938	1.00 25.22	A
	ATOM	1387	CB	ALA A 246	43.247	33.675	13.867	1.00 23.27	A
		2001	CD	DUD N 240	42.956	34.955	13.082	1.00 22.94	A

	ATOM	1388	С	ALA Z	246	42.178	33.475	14.934	1.00 21.27	70
	ATOM	1389	ō	ALA A		42.431	•			A
	ATOM	1390	N	GLN A				16.114	1.00 20.93	· A
						40.988	33.047	14.536	1.00 19.67	A
-	ATOM	1391	CA	GLN A		39.911	32.886	15.504	1.00 20.17	A
5	MOTA	1392	CB	GLN A		38.608	32.535	14.779	1.00 21.89	A
	MOTA	1393	CG	GLN A	247	38.522	33:076	13.355	1.00 26.18	A
	ATOM	1394	CD	GLN A	247	37.220	33.794	13.064	1.00 27.30	· A
	ATOM	1395	OE:	l GLN A	247	36.172	33.447	13.605	1.00 30.13	A
	ATOM	1396		GLN A		37.278	34.792	12.189	1.00 28.70	A
10	ATOM	1397	С	GLN A		40.181	31.849	16.595	1.00 19.43	A
	ATOM	1398	ō	GLN A		39.546	31.883	17.648		
	ATOM	1399	N	TYR A					1.00 18.93	A
							30.948	16.359	1.00 18.60	A
	MOTA	1400		TYR A		41.441	29.896	17.329	1.00 19.20	A
16	MOTA	1401	CB	TYR A		41.333	28.529	16.642	1.00 17.53	A
15	MOTA	1402	CG	TYR A		40.013	28.362	15.927	1.00 19.32	Α
	ATOM			L TYR A		38.859	28.010	16.625	1.00 17.69	A
	ATOM	1404		L TYR A		37.617	27.976	15.990	1.00 18.18	А
	ATOM	1405	CD2	TYR A	248	39.897	28.664	14.569	1.00 16.87	A
	ATOM	1406	CE2	TYR A	248	38.665	28.635	13.924	1.00 19.17	A
20	ATOM	1407	CZ	TYR A		37.527	28.295	14.643	1.00 19.46	A
	ATOM	1408	ОН	TYR A		36.299	28.311	14.023	1.00 18.98	
	ATOM	1409	С	TYR A		42.810	30.039	17.993	1.00 20.42	A
	ATOM	1410	Ö	TYR A		43.208	29.191	18.792	1.00 20.42	
	ATOM	1411	N	VAL A		43.523	31.114			A
25	ATOM	1412					•	17.673	1.00 20.20	A
23			CA	VAL A		44.841	31.343	18.251	1.00 20.91	A
	ATOM	1413	CB	VAL A		45.542	32.532	17.570	1.00 21.18	A
	ATOM	1414		VAL A		46.821	32.896	18.317	1.00 22.45	A
	ATOM	1415		VAL A		45.862	32.170	16.139	1.00 24.01	Α
	ATOM	1416	С	VAL A	249	44.764	31.606	19.750	1.00 21.52	Α
30	ATOM	1417	0	VAL A		43.915	32.368	20.216	1.00 22.72	A
	ATOM	1418	N.	SER A	250	45.654	30.965	20.503	1.00 20.70	A
	ATOM	1419	CA	SER A	250	45.697	31.133	21.951	1.00 21.65	Α
	ATOM	1420	CB	SER A	250	46.370	29.919	22.613	1.00 22.02	A
	ATOM	1421	OG	SER A	250	47.692	29.725	22.132	1.00 22.12	A
35	ATOM	1422	С	SER A		46.476	32.402	22.280	1.00 22.13	A
	ATOM	1423	ō	SER A		47.332	32.828	21.511	1.00 22.77	A
	ATOM	1424	N	PRO A		46.180	33.029	23.425	1.00 22.77	Ā
	ATOM	1425	CD	PRO A		45.163				
	ATOM	1426					32.684	24.433	1.00 22.97	A
40			CA	PRO A		46.893	34.254	23.800	1.00 22.52	A
40	ATOM	1427	CB	PRO A		46.233	34.650	25.127	1.00 23.06	A
	ATOM	1428	CG	PRO A		45.726	33.329	25.676	1.00 22.55	A
	ATOM	1429	С	PRO A		48.414	34.115	23.907	1.00 22.15	A
	ATOM	1430	0	PRO A		49.143	35.047	23.563	1.00 22.62	A
	ATOM	1431	N	GLU A		48.901	32.966	24.367	1.00 20.69	Α
45	MOTA	1432	CA	GLU A	252	50:347	32.772	24.500	1.00 21.40	A
	MOTA	1433	CB	GLU A	252	50.673	31.382	25.071	1.00 20.59	A
	ATOM	1434	CG	GLU A	252	49.993	30.232	24.352	1.00 21.91	A
	ATOM	1435	CD	GLU A		48.691	29.822	25.014	1.00 21.51	A
	ATOM	1436		GLU A		47.989	30.707	25.550	1.00 21.46	A
50	ATOM	1437		GLU A		48.367	28.613	24.993	1.00 20.23	A
	ATOM	1438	С	GLU A		51.071	32.970		1.00 20.23	
	MOTA	1439	0	GLU A		52.191		23.167	1.00 22.99	A
										A
	ATOM	1440	N	LEU A		50.441	32.576	22.064	1.00 23.00	A
e e	ATOM	1441	CA	LEU A		51.068	32.753	20.758	1.00 25.62	A
55	MOTA	1442	CB	LEU A		50.277	32.029	19.669	1.00 26.75	A
	ATOM	1443	CG	LEU A		50.743	30.620	19.296	1.00 31.87	A
	MOTA	1444		LEU A		50.433	29.651	20.422	1.00 31.81	A
	MOTA	1445	CD2	LEU A	253	50.044	30.179	18.015	1.00 31.86	Α
	MOTA	1446	С	LEU A	253	51.201	34.228	20.371	1.00 26.94	A

	ATOM	1447	0	LE	JA	253		52.107	34.601	19.626	1.00 27.09	А
	ATOM	1448	N	LE	JA	254		50.297	35.059			
	ATOM	1449	CA	LE	JA	254		50.297	36.485	20.564	1.00 27.26	
	ATOM	1450	CB	LE	AC	254		48.858	37.006		1.00 25.84	A
5	ATOM	1451	CG	LE	JA	254		47.882	36.290	19.621	1.00 24.69	Ą.
	ATOM	1452	CD	1 LE	JΑ	254		46.459	36.724	19.932	1.00 23.64	Ā
	ATOM	1453		2 LEC				48.236	36.597	18.177	1.00 23.04	
	' ATOM	1454	C.			254		51.134	37.314	21.537	1.00 24.24	A
	ATOM	1455	Ō			254		51.633	38.383	21.187	1.00 30.02	A
10	ATOM	1456	N			255		51.292	36.821	22.758	1.00 32.33	A
	ATOM	1457	CA			255		52.056	37.547	23.759	1.00 32.47	A
	ATOM	1458	CB			255		51.368	37.478	25.127	1.00 36.70	A
	ATOM	1459		1 THE				51.188	36.106	25.494	1.00 34.31	A
	ATOM	1460		2 THE				50.013	38.166	25.077	1.00 33.49	A
15	ATOM	1461	C			255		53.477	37.035	23.910	1.00 33.40	A
	ATOM	1462	o			255		54.430	37.793	23.772		A
	ATOM	1463	N			256		53.617	35.747	24.189	1.00 43.69	A
	ATOM	1464	CA			256		54.932	35.144	24.189	1.00 44.77 1.00 49.15	A
	ATOM	1465	CB			256		54.866	34.143	25.534	1.00 49.15	A
20	ATOM	1466	CG			256		54.514	34.786	26.862		A
	ATOM	1467	CD			256		54.053	33.780	27.893	1.00 56.03	A
	ATOM	1468		LGLU				54.766	32.776	28.107	1.00 58.83 1.00 62.13	A
	ATOM	1469		GLU				52.979	33.996	28.494	1.00 60.34	A
	ATOM	1470	C C			256		55.475	34.456	23.137	1.00 50.09	A A
25	ATOM	1471	ō			256		56.616	33.995	23.127	1.00 50.42	A
	ATOM	1472	N			257		54.658	34.389	22.090	1.00 50.42	A
	ATOM	1473	CA			257		55.064	33.746	20.845	1.00 51.21	A
	ATOM	1474	СВ			257		56.244	34.502	20.227	1.00 51.22	A
	ATOM	1475	CG			257		56.558	34.125	18.790	1.00 55.19	A
30	MOTA	1476	CD			257		57.709	34.961	18.253	1.00 57.52	Α.
	ATOM	1477	CE			257		57.952	34.694	16.777	1.00 58.52	A
	ATOM	1478	NZ	LYS	Α	257		58.290	33.268	16.515	1.00 60.88	A
	ATOM	1479	С	LYS	Α	257		55.467	32.302	21.138	1.00 50.74	A
	ATOM	1480	0	LYS	A	257		56.432	31.790	20.577		A
35	ATOM	1481	N	SER	A	258		54.721	31.654	22.027	1.00 48.07	A
	MOTA	1482	CA	SER	Α	258		54.999	30.273	22.402	1.00 46.87	A
	ATOM	1483	CB	SER	A	258	•	55.590	30.229	23.812	1.00 48.88	A
•	ATOM	1484	OG	SER	A	258		54.741	30.892	24.734	1.00 53.14	A
	ATOM	1485	С	SER	A	258		53.735	29.415	22.342	1.00 44.07	A
40	ATOM	1486	0	SER	Α	258		52.617	29.932	22.417	1.00 44.17	Α
	MOTA	1487	N	ALA	Α	259		53.917	28.105	22.204	1.00 38.30	Α
	ATOM	.1488	CA	ALA	Α	259		52.793	27.180	22.127	1.00 34.73	· A
	MOTA	1489	CB	ALA	Α	259		52.551	26.779	20.684	1.00 34.16	A
	ATOM .	1490	С	ALA	Α	259		53.042	25.940	22.977	1.00 32.34	A
45	ATOM	1491	0	ALA				54.172	25.459	23.086	1.00 31.81	A
	ATOM	1492	N	CYS				51.975	25.428	23.579	1.00 28.58	Α.
	ATOM	1493	CA	CYS			•	52.056	24.244	24.425	1.00 26.27	Α
	ATOM	1494	CB	CYS				52.183	24.654	25.892	1.00 26.53	A
	ATOM	1495	SG	CYS				50.846	25.739	26.469	1.00 32.91	А
50	ATOM	1496	С	CYS				50.786	23.435	24.224	1.00 22.83	Α
	ATOM	1497	0	CYS				49.892	23.856	23.495	1.00 22.14	A
	ATOM	1498	N	LYS				50.706	22.277	24.868	1.00 20.02	A
	ATOM	1499	CA	LYS				49.526	21.434	24.744	1.00 20.65	Α
c c	ATOM	1500	CB	LYS				49.619	20.243	25.696	1.00 23.28	A
55	ATOM	1501	CG	LYS				50.716	19.253	25.347	1.00 27.44	A
	MOTA	1502	CD	LYS				50.732	18.117	26.350	1.00 29.98	A
	ATOM	1503	CE	LYS				51.922	17.203	26.134	1.00 32.34	A
	ATOM	1504	NZ	LYS				51.940	16.121	27.153	1.00 33.28	A
	ATOM	1505	С	LYS	Α	261		48.268	22.229	25.062	1.00 19.20	A

	ATOM	1506	0	LYS A	261	47.253	22.092	24.387	1,00 18.0	ת פר
	ATOM	1507	N	SER A	262	48.358				
	ATOM	1508	CA	SER A		47.235				
	ATOM	.1509	CB	SER A		47.644			1.00 18.2	
5	ATOM	1510		SER A		46.517		28.421		
	ATOM	1511		SER A		46.736				
	ATOM	1512		SER A		45.591				
•	ATOM	1513		SER A		47.595				
	ATOM	1514		SER A						
10	ATOM	1515		SER A		47.175	25.970	23.347		
	ATOM	1516				48.340	26.228	22.382		
	ATOM	1517		SER A		49.402	26.909	23.031		
	ATOM		C	SER A		46.040	25.257	22.612	1.00 17.7	9 A
		1518	0	SER A		45.099	25.898	22.148	1.00 17.5	
15	ATOM	1519		ASP A		46.119	23.928	22.517	1.00 16.3	0 A
15	ATOM	1520		ASP A		45.069	23.166	21.836	1.00 16.7	2 A
	ATOM	1521		ASP A		45.483	21.704	21.620	1.00 15.9	2 A
	ATOM	1522		ASP A		46.544	21.539	20.548	1.00 17.9	
	ATOM	1523		ASP A		46.642	22.412	19.661	1.00 16.7	
	ATOM	1524		ASP A		47.265	20.515	20.579	1.00 16.6	
20	ATOM	1525	C	ASP A	264	43.773	23.194	22.646	1.00 17.6	
	MOTA	1526	0	ASP A	264	42.681	23.197	22.076	1.00 18.2	
	ATOM	1527	N	LEU A	265	43.898	23.205	23.974	1.00 15.4	
	MOTA	1528	CA	LEU A	265	42.730	23.232	24.849	1.00 14.7	
	ATOM	1529	CB :	LEU A	265	43.147	23.038	26.313	1.00 11.3	
25	ATOM	1530		LEU A		43.711	21.641	26.621	1.00 14.0	
	ATOM	1531		LEU A		44.249	21.579	28.052	1.00 13.9	
	ATOM	1532		LEU A		42.619	20.603	26.416	1.00 13.9	
	ATOM	1533		LEU A		41.999	24.557	24.675	1.00 11.0	
	ATOM	1534		LEU A		40.777	24.620	24.785		
30	ATOM	1535		TRP A		42.746	25.622		1.00 16.75	
	ATOM	1536		TRP A		42.118		24.405	1.00 16.08	
	ATOM	1537		TRP A			26.918	24.184	1.00 16.96	
	ATOM	1538		TRP A		43.176	28.015	24.023	1.00 17.28	
	ATOM	1539		TRP A		42.618	29.326	23.521	1.00 20.54	
35	ATOM	1540		TRP A		42.313	30.490	24.301	1.00 20.07	
-	ATOM	1541		RP A		41.782	31.459	23.417	1.00 20.46	
	ATOM	1542		RP A		42.435	30.810	25.660	1.00 20.68	
	ATOM	1543		RP A		42.270	29.631	22.231	1.00 19.53	
	ATOM	1543	NET 1	IRP A	200	41.769	30.908	22.163	1.00 19.61	
40	ATOM	1545	.042 1	RP A	200 0.66	41.372	32.727	23.850	1.00 20.90	
70	ATOM	1545		RP A		42.026	32.073	26.091	1.00 19.45	
		1546		RP A		41.501	33.015	25.185	1.00 20.71	
	ATOM			RP A		41.284	26.795	22.913	1.00 17.22	A
	MOTA	1548		RP A		40.139	27.240	22.863	1.00 18.03	A
15	ATOM	1549		LA A		41.863	26.181	21.886	1.00 17.50	A
45	ATOM	1550		LA A		41.155	25.990	20.626	1.00 16.16	A
	ATOM	1551		LA A 2		42.050	25.290	19.621	1.00 14.28	A
	ATOM	1552		LA A 2		39.901	25.159	20.891	1.00 16.28	
	ATOM .	1553		LA A 2		38.835	25.436	20.346	1.00 16.46	
	ATOM	1554	N L	EU A 2	268	40.031	24.144	21.739	1.00 16.57	
50	ATOM	1555		EU A 2		38.890	23.299	22.084	1.00 17.03	A
	ATOM	1556	CB L	EU A 2	268	39.292	22.260	23.139	1.00 15.35	A
	ATOM	1557	CG L	EU A 2	68	38.158	21.429	23.754	1.00 19.00	A
	ATOM	1558		EU A 2		37.505	20.578	22.678	1.00 15.00	A
	ATOM	1559		EU A 2		38.718	20.537	24.881	1.00 10.17	
55	ATOM	1560		EU A 2		37.766	24.179	22.628	1.00 17.49	\ A
	ATOM	1561		EU A 2		36.603	24.179	22.247	1.00 15.72	A
	ATOM	1562		LY A 2		38.119	25.099	23.520	1.00 15.28	A
	ATOM	1563		LY A 2		37.124				A
	ATOM	1564		LY A 2		36.406	25.989	24.092	1.00 13.39	A
			J J.	41 2		20.400	26.808	23.031	1.00 14.94	Α

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	MOTA				A 269		35.193	3 27.014	23.11	1 1.0	0 14.76	A
	MOTA			CYS	A 270		37.146				0 13.86	
	ATOM	1567	7 CA	CYS	A 270		36.539				0 16.80	
	ATOM	1568	3 CB	CYS .	A 270		37.611				0 15.97	
5	ATOM	1569	SG	CYS .	A 270		38.751				0 20.48	
	ATOM	1570) C		A 270		35.598				0 20.48	
	ATOM	1571	. 0		A 270		34.516					
	ATOM	1572	. N		A 271		36.022				0 18.38	
	ATOM	1573	CA		A 271		35.221				0 16.99	
10	ATOM	1574			A 271		36.038				0 16.66	
	ATOM	1575		ILE A			35.155	23.741			0 16.53	
	ATOM	1576		ILE A							0 16.34	A
	ATOM	1577	CD1	ILE A	7 2/1 7 271		37.222				0 15.59	A
	ATOM	1578			A 271		38.239				0 14.88	A
15	ATOM	1579		ILE A	1 2/1		33.920				16.74	· A
13	ATOM	1580					32.865				17.12	A
	ATOM			ILE A			33.990				16.13	A
	ATOM	1581		ILE A			32.785				18.30	A
		1582		ILE F			33.097			1.00	17.77	A
20	ATOM	1583		ILE A			31.796	23.666	24.152	1.00	17.96	A
20	ATOM	1584		ILE A			33.877	22.437	23.481		19.55	A
	MOTA	1585		ILE A			34.446	22.217	24.886		18.64	A
	ATOM	1586	С	ILE A			31.824	25.207	21.776		19.51	A
	ATOM	1587	0	ILE A			30.624	25.037	21.554		20.44	A
	ATOM	1588	N	TYR A			32.362	26.409	21.947	1.00	18.52	A
25	ATOM	1589	CA	TYR A		-	31.553	27.615	21.881		20.48	A
	MOTA	1590	CB	TYR A			32.418	28.847	22.162		18.98	A
	ATOM	1591	CG	TYR A	273		31.663	30.161	22.125		20.26	A
	ATOM	1592	CD1	TYR A			31.229	30.709	20.916		20.67	A
	ATOM	1593	CE1	TYR A	273		30.536	31.917	20.880		20.98	A
30	ATOM	1594	CD2	TYR A	273		31.383	30.857	23.302		19.82	A
*	ATOM	1595		TYR A			30.691	32.062	23.280		20.62	A
	ATOM	1596	CZ	TYR A			30.271	32.587	22.067		21.15	
	ATOM	1597	ОН	TYR A			29.588	33.776	22.049		21.15	A
	ATOM	1598	С	TYR A		-	30.902	27.730	20.507		21.54	A
35	ATOM	1599	0	TYR A			29.719	28.049	20.401		22.80	A
	ATOM	1600	N	GLN A			31.676	27.454	19.461		21.05	· A
	ATOM	1601	CA	GLN A			31.176	27.538	18.095		21.03	A
	MOTA	1602		GLN A			32.323	27.341	17.097		21.46	A
	ATOM	1603		GLN A			31.934	27.596	15.645			A
40	ATOM	1604		GLN A			33.131	27.588	14.706		23.15	A
	ATOM	1605		GLN A			34.276	27.446	15.139		24.80	A
	ATOM	1606		GLN A			32.870	27.750			22.51	A
	ATOM	1607		GLN A			30.076	26.517	13.413 17.828		22.96	A
	ATOM	1608		GLN A			29.123	26.806			21.51	A
45	ATOM	1609		LEU A			30.207		17.108		20.50	A
	ATOM	1610		LEU A			29.196	25.324	18.403		21.44	A
	ATOM	1611		LEU A				24.282	18.208		20.95	A
	ATOM	1612		LEU A			29.645 30.775	22.958	18.846		19.11	A
	ATOM	1613		LEU À				22.182	18.159		21.43	A
50	ATOM	1614					31.118	20.936	18.963		17.64	А
	ATOM	1615		LEU A			30.342	21.795	16.754		20.34	A.
	ATOM			LEU A			27.860	24.697	18.815		21.32	A
	ATOM	1616 1617		LEU A			26.802	24.461	18.229		19.75	Α
	ATOM	1617		VAL A			27.921	25.322	19.987		19.10	A
55	ATOM	1618		VAL A			26.724	25.750	20.702		22.47	A
55		1619		/AL A			27.011	25.882	22.217	1.00	20.87	A
	ATOM	1620		/AL A			25.742	26.291	22.957	1.00	19.68	Α
	ATOM	1621		/AL _. A			27.550	24.558	22.766	1.00	19.43	A
	ATOM	1622		AL A			26.127	27.075	20.211	1.00	23.89	A
	ATOM	1623	0 1	AL A	276	- 2	24.910	27.199	20.070	1.00	24.90	A
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	ATOM	1624	N	ALA A 2		26.983	28.062	19.965	1.00 24.56	A
	ATOM	1625	CA	ALA A 2	77	26.533	29.374	19.518	1.00 24.72	А
	ATOM	1626	CB	ALA A 2	77	27.504	30.444	19.999	1.00 24.36	A
	ATOM	1627	С	ALA A 2	77	26.378	29.458	18.005		A
5	ATOM	1628	0	ALA A 2	77	25.577	30.242	17.502	1.00 26.39	A
	MOTA	1629	N	GLY A 2	78	27.142	28.651	17.280	1.00 25.13	A
	MOTA	1630	CA	GLY A 2	78	27.062	28.673	15.834	1.00 25.58	A
	MOTA	1631	С	GLY A 2	78	28.163	29.524	15.231	1.00 26.50	A
	ATOM	1632	0	GLY A 2		28.374	29.510	14.015	1.00 28.17	A
10	ATOM	1633	N	LEU A 2		28.866	30.262	16.086	1.00 24.44	A
	ATOM	1634	CA	LEU A 2		29.962	31.130	15.656	1.00 24.44	A
	ATOM	1635	CB	LEU A 2		29.468	32.575	15.500	1.00 25.78	A
	ATOM	1636	CG	LEU A 2		28.364	32.899	14.490	1.00 23.78	
	ATOM	1637		L LEU A 2		27.922	34.344	14.684		A
15	ATOM	1638		FEU A 2		28.862	32.670		1.00 26.60	A
	ATOM	1639	C	LEU A 2		31.093		13.071	1.00 26.52	A
	ATOM	1640	Ö	LEU A 2			31.116	16.687	1.00 23.47	A
	ATOM	1641	N	PRO A 28		30.848	30.994	17.882	1.00 24.44	A
	ATOM	1642	CD	PRO A 28		32.349	31.239	16.236	1.00 23.35	A
20	ATOM					32.831	31.404	14.855	1.00 22.26	A
20		1643	CA	PRO A 28		33.464	31.239	17.189	1.00 23.81	A
	ATOM	1644	CB	PRO A 28		34.692	31.293	16.282	1.00 23.24	A
	ATOM	1645	CG	PRO A 28		34.189	32.020	15.073	1.00 24.89	A
	ATOM	1646	С	PRO A 28		33.353	32.444	18.137	1.00 22.69	A
05	ATOM	1647	0	PRO A 28		32.750	33.457	17:788	1.00 22.11	A
25	MOTA	1648	N	PRO A 28		33.939	32.344	19.345	1.00 23.06	A
	ATOM	1649	CD	PRO A 28		34.810	31.223	19.734	1.00 21.37	A
	ATOM	1650	CA	PRO A 28		33.935	33.375	20.395	1.00 23.67	A
	ATOM	1651	CB	PRO A 28		34.781	32.751	21.509	1.00 24.89	A
	ATOM	1652	CG	PRO A 28		34.749	31.287	21.219	1.00 25.24	. A
30	ATOM	1653	С	PRO A 28		34.481	34.752	20.017	1.00 23.75	A
	ATOM	1654	0	PRO A 28		33.869	35.781	20.317	1.00 21.02	A
	ATOM	1655	N	PHE A 28		35.644	34.763	19.379	1.00 22.17	A
	MOTA	1656	CA	PHE A 28		36.293	36.007	18.998	1.00 23.16	A
2.1	ATOM	1657	CB	PHE A 28		37.765	35.943	19.406	1.00 21.01	A
35	ATOM	1658	CG	PHE A 28		37.975	35.482	20.822	1.00 22.66	A
	ATOM	1659	CD1	PHE A 28	2	37.806	36.361	21.888	1.00 20.06	A
	MOTA	1660		PHE A 28		38.291	34.151	21.093	1.00 20.72	A
	ATOM	1661	CE1	PHE A 28	2	37.947	35.921	23.206	1.00 22.66	A
	ATOM	1662	CE2	PHE A 28	2	38.433	33.702	22.405	1.00 20.97	A
40	ATOM	1663	CZ	PHE A 28	2	38.261	34.590	23.466	1.00 19.58	A
	ATOM	1664	С	PHE A 28	2	36.169	36.263	17.503	1.00 24.39	A
	ATOM	1665	0	PHE A 28	2	36.802	35.585	16.694	1.00 25.80	A
	ATOM	1666	N	ARG A 28	3	35.355	37.248	17.142	1.00 24.99	A
	ATOM	1667	CA	ARG A 28	3	35.141	37.594	15.741	1.00 26.33	A
45	ATOM	1668	CB	ARG A 28	3	33.721	37.209	15.316	1.00 28.91	A
	ATOM	1669	CG	ARG A 28	3	33.293	35.808	15.724	1.00 30.27	А
	ATOM	1670	CD	ARG A 28	3	31.904	35.493	15.188	1.00 33.36	A
	ATOM	1671	NE	ARG A 28	3	30.890	36.392	15.733	1.00 32.76	Α
	MOTA	1672	CZ	ARG A 28	3	30.372	36.287	16.952	1.00 34.79	А
50	ATOM	1673	NH1	ARG A 28	3	30.767	35.317	17.768	1.00 35.77	A
	ATOM	1674	NH2	ARG A 28	3	29.458	37.156	17.359	1.00 36.12	А
	ATOM	1675	С	ARG A 28		35,328	39.096	15.544	1.00 26.47	A
	ATOM	1676	0	ARG A 28		35.029	39.888	16.438	1.00 26.28	A
	ATOM	1677	N	ALA A 28		35.818	39.486	14.373	1.00 26.70	A
55	ATOM	1678	CA	ALA A 28		36.033	40.899	14.079	1.00 27.84	A
	ATOM	1679	CB	ALA A 28		37.188	41.442	14.914	1.00 26.24	A
	ATOM	1680	C	ALA A 28		36.327	41.077	12.602	1.00 28.35	A
	ATOM	1681	ō	ALA A 28		36.560	40.101	11.891	1.00 29.91	A
	ATOM	1682	N	GLY A 28		36.332	42.329	12.153	1.00 29.29	A
					-	00.002		,		L.

	ATOM	1683	CA	GLY	A 2	85	3	6.577	42.631	10.753	3 1 00	29.52	A
	ATOM	1684	С	GLY	A 2	85		7.893	42.156			30.12	Ä
	ATOM	1685	0	GLY			3.	7.974	41.862			30.60	A
	ATOM	1686	N	ASN	A 2	86	38	3.939	42.097	10.983		28.49	A
5	ATOM	1687	CA	ASN	A 2	86	40	0.231	41.644	10.489		26.71	A
	ATOM	1688	СВ	ASN				1.050	42.825	9.945		26.11	A
	MOTA	1689	CG	ASN	A 2	86		1.310	43.900	10.990		27.83	A
	MOTA	1690	OD:	L ASN				1.877	43.631	12.049		27.84	A
	ATOM	1691		2 ASN				908	45.131	10.685		25.95	A
10	ATOM	1692	С	ASN	A 2	86		0.997	40.924	11.584		26.03	A
	ATOM	1693	0	ASN).540	40.851	12.723		25.66	A
	MOTA	1694	N	GLU				2.162	40.391	11.239		24.81	A
	MOTA	1695	CA	GLU	A 2	87	42	2.965	39.662	12.206		27.59	A
	MOTA	1696	СВ	GLU				.145	38.985	11.510		30.17	A
15	ATOM	1697	CG	GLU				3.776	37.632	10.931		38.21	A
	ATOM	1698	CD	GLU				.900	36.998	10.140		41.86	A
	ATOM	1699		GLU				.061	37.036	10.608		43.08	A
	ATOM	1700		GLU				.612	36.449	9.052		45.22	A
	ATOM	1701	C	GLU				3.459	40.485	13.383		25.05	A
20	ATOM	1702	ō	GLU				.382	40.030	14.521		26.41	A
	ATOM	1703	N	TYR				.966	41.685	13.122		23.04	A
	ATOM	1704	CA	TYR				.460	42.528	14.205		22.34	A
	ATOM	1705	СВ	TYR				.867	43.913	13.691		21.07	A
	MOTA	1706	CG	TYR				.275	44.858	14.805		21.07	A
25	ATOM	1707		TYR				.533	44.762	15.405		21.23	A
	ATOM	1708	CE1					.891	45.588	16.475		20.43	A
	ATOM	1709		TYR				.380	45.809	15.302		22.32	A
~	ATOM	1710		TYR				.725	46.637	16.373		23.28	A
	ATOM	1711	CZ	TYR				.981	46.518	16.953		22.96	. A
30	ATOM	1712	OH	TYR				.316	47.313	18.024		23.18	A
	ATOM	1713	C	TYR				.402	42.698	15.288		21.38	A
	ATOM	1714	ō	TYR				.710	42.616	16.473		22.09	A
	ATOM	1715	N	LEU				.159	42.939	14.874		21.88	A
	ATOM	1716	CA	LEU				.055	43.130	15.811		21.98	A
35	ATOM	1717	СВ	LEU				.821	43.673	15.078		22,90	A
	ATOM	1718	CG	LEU .				.896	45.130	14.601		26.52	A
	ATOM '	1719	CD1					.706	45.436	13.696		26.55	A
	ATOM	1720	CD2	LEU .				.914	46.071	15.807		23.13	A
	ATOM	1721	С	LEU .				.686	41.849	16.560		21.24	A
40	ATOM	1722	0	LEU .				.256	41.897	17.715		20.72	A
	ATOM	1723	N	ILE				.843	40.708	15.900		19.62	A
	ATOM	1724	CA	ILE :				.538	39.433	16.533		18.54	A
	ATOM	1725	CB	ILE :				.560	38.281	15.509		18.52	A
	ATOM	1726	CG2	ILE :	A 29	0		.503	36.934	16.234		17.63	A
45	ATOM	1727	CG1	ILE A	A 29	0		.378	38.429	14.545		18.88	A
	ATOM	1728		ILE 2				.421	37.483	13.357		19.81	A
	ATOM	1729	С	ILE A				.578	39.167	17.618		19.09	A
	MOTA	1730	0	ILE A				.236	38.788	18.737		18.20	A
	MOTA	1731	N	PHE 2				.849	39.376	17.286	1.00	18.76	A
50	ATOM	1732	CA	PHE Z			43	.925	39.156	18.247		20.75	A
	ATOM	1733	CB	PHE 2				.286	39.434	17.606		20.71	. A
	MOTA	1734	CG	PHE A			45	. 644	38.480	16.503	1.00	22.92	A
	ATOM	1735	CD1	PHE A	A 29	1	45	.065	37.214	16.443		22.98	A
	MOTA	1736		PHE Z				.588	38.830	15.543		22.91	A
55	ATOM	1737		PHE A				.423	36.310	15.440		24.51	A
	ATOM	1738		PHE A				.954	37.931	14.535		25.54	A
	ATOM	1739	CZ	PHE A				.370	36.670	14.485		23.29	A
	ATOM	1740	С	PHE A				.739	40.061	19.451		21.72	A
	ATOM	1741	0	PHE A				. 992	39.671	20.593		22.32	A

	ATOM	1742	N	GLN A	292		43.284	41.275	19.178	1.00 23.27	70
	ATOM	1743	CA			•	43.055	42.264	20.216	1.00 23.27	
	ATOM	1744	СВ	GLN A			42.574	43.559			A
	ATOM	1745	CG	GLN A			42.577	44.773	19.562	1.00 25.77	A
5	ATOM	1746	CD						20.447	1.00 28.45	A
,				GLN A			42.469	46.057	19.638	1.00 29.83	Α
	ATOM	1747		1 GLN A			41.520	46.244	18.872	1.00 27.16	A
	ATOM	1748	NE:				43.449	46.944	19.799	1.00 27.61	Α
	ATOM	1749	С	GLN A			42.018	41.733	21.204	1.00 22.97	Α
	ATOM	1750	0	GLN A	292		42.200	41.832	22.415	1.00 21.64	A
10	ATOM	1751	N	LYS A	293		40.937	41.154	20.687	1.00 21.82	A
	ATOM	1752	CA	LYS A	293		39.895	40.612	21.558	1.00 22.18	A
	ATOM	1753	СВ	LYS A			38.664	40.223	20.740	1.00 22.69	A
	ATOM	1754	CG	LYS A			37.919	41.407	20.153	1.00 25.78	A
	ATOM	1755	, CD	LYS A			36.651	40.961			
15	ATOM	1756	CE	LYS A			35.857		19.429	1.00 27.88	A
13	ATOM	1757	NZ					42.161	18.926	1.00 30.85	A
				LYS A			34.612	41.750	18.214	1.00 32.98	Α
	ATOM	1758	C	LYS A			40.398	39.398	22.343	1.00 21.20	A
	MOTA	1759	0	LYS A			40.041	39.204	23.509	1.00 22.01	А
	ATOM	1760	N	ILE A			41.226	38.583	21.702	1.00 19.91	A
20	MOTA	1761	CA	ILE A			41.774	37.394	22.347	1.00 20.28	A
	MOTA	1762	CB	ILE A			42.631	36.575	21.349	1.00 18.98	A
	ATOM	1763	CG2	ILE A	294		43.481	35.550	22.098	1.00 17.70	A
	MOTA	1764	CG1	ILE A	294		41.716	35.897	20.318	1.00 17.93	A
	ATOM	1765	CD1	. ILE A	294		42.467	35.237	19.178	1.00 16.21	A
25	ATOM	1766	С	ILE A	294		42.618	37.727	23.587	1.00 21.94	A
	ATOM	1767	0	ILE A	294		42.366	37.199	24.673	1.00 20.86	A
	MOTA	1768	N	ILE A			43.610	38.600	23.439	1.00 21.88	A
	ATOM	1769	CA	ILE A			44.461	38.934	24.582	1.00 24.25	A
	ATOM	1770	CB	ILE A			45.668	39.805	24.175	1.00 23.93	A
30	ATOM	1771		ILE A			46.514	39.066	23.140	1.00 23.93	A
30	ATOM	1772		ILE A			45.189	41.151	23.637		
	MOTA	1773		ILE A						1.00 24.58	A
							46.317	42.149	23.433	1.00 26.69	A
	ATOM	1774	С	ILE A			43.720	39.636	25.717	1.00 24.80	A
25	ATOM	1775	0	ILE A			44.214	39.687	26.842	1.00 24.76	A
35	ATOM	1776	N	LYS A			42.539	40.173	25.425	1.00 25.33	A
	ATOM	1777	CA	LYS A			41.743	40.853	26.444	1.00 26.80	A
	MOTA	1778	CB	LYS A			41.178	42.170	25.894	1.00 27.39	A
	ATOM	1779	CG	LYS A	296		42.240	43.141	25,413	1.00 31.79	Α
	MOTA	1780	CD	LYS A			41.634	44.410	24.826	1.00 35.56	A
40	ATOM	1781	CE	LYS A	296		41.009	45.283	25.900	1.00 39.29	A
	ATOM	1782	NZ	LYS A	296		40.564	46.603	25.357	1.00 41.72	A
	MOTA	1783	С	LYS A	296		40.593	39.958	26.893	1.00 25.50	A
	MOTA	1784	0	LYS A	296		39.770	40.361	27.713	1.00 24.02	A
	ATOM	1785	N	LEU A	297		40.550	38.742	26.349	1.00 25.67	A
45	ATOM	1786	CA	LEU A			39.500	37.777			A
	ATOM	1787	СВ	LEU A			39.632	37.285	28.111	1.00 24.80	A
	ATOM	1788	CG	LEU A			38.766	36.068	28.460	1.00 24.00	A
	ATOM	1789		LEU A			39.238		27.646	1.00 26.70	
	ATOM	1790		LEU A			38.856	34.852 35.777			A
50	ATOM	1791		LEU A					29.951	1.00 24.84	A
50			C				38.151	38.459	26.467	1.00 25.11	A
	ATOM	1792	0	LEU A			37.261	38.378	27.309	1.00 25.28	A
	ATOM	1793	N	GLU A			38.007	39.127	25.331	1.00 24.98	A
	ATOM	1794	CA	GLU A			36.786	39.847	25.023	1.00 25.31	A
	ATOM	1795	CB	GLU A			37.143	41.139	24.291	1.00 27.13	A
55	ATOM	1796	CG	GLU A			35.991	42.092	24.108	1.00 31.28	A
	MOTA	1797	CD	GLU A			36.419	43.362	23.410	1.00 34.40	A
	MOTA	1798		GLU A			37.348	44.027	23.918	1.00 35.90	A
	ATOM	1799	OE2	GLU A	298		35.832	43.693	22.359	1.00 36.16	A
	ATOM	1800	С	GLU A	298		35.766	39.057	24.207	1.00 23.79	A

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	ATOM	1801	. 0	GLU A	298	35.832	39.017	22.979	1.00 24.35	5 70
	ATOM	1802		TYR A		34.825				
	ATOM	1803				33.760				-
	ATOM	1804		TYR A		34.264				
5	ATOM	1805								
,						34.348				
	ATOM	1806		1. TYR A		35.336			1.00 19.32	2 A
	ATOM	1807		1 TYR A		35.389			1.00 19.30) A
	ATOM	1808		2 TYR A		33.410	34.201	24.888	1.00 18.96	
	ATOM	1809		2 TYR A		33.456	33.243	25.907	1.00 19.41	
10	ATOM	1810	CZ	TYR A	299	34.449	33.321	26.870		
	ATOM	1811	OH	TYR A	299	34.511	32.401	27.881		
•	MOTA	1812	С	TYR A	299	32.699		25.331		
	MOTA	1813	0	TYR A	299	32.942	37.681	26.506		
	ATOM	1814	N	ASP A		31.522	36.981	24.927		
15	ATOM	1815	CA	ASP A		30.467	36.710	25.891		
	ATOM	1816	СВ	ASP A		29.665	37.981		1.00 30.60	
	ATOM	1817	CG	ASP A				26.179	1.00 35.86	
	ATOM	1818		ASP A		29.228	38.687	24.923	1.00 42.04	
	ATOM	1819		ASP A :		28.450	38.088	24.149	1.00 45.98	
20	ATOM	1820				29.666	39.840	24.707	1.00 45.69	
20			С	ASP A		29.564	35.608	25.363	1.00 29.26	A
	ATOM	1821	0	ASP A		29.590	35.299	24.172	1.00 28.64	Α
	ATOM	1822	N	PHE A		28.778	35.011	26.253	1.00 28.96	Α
	ATOM	1823	CA	PHE A		27.884	33.924	25.871	1.00 30.48	A
	MOTA	1824	CB	PHE A 3		27.818	32.854	26.968	1.00 29.17	A
25	ATOM	1825	CG	PHE A 3		29.147	32.279	27.356	1.00 29.29	A
	ATOM	1826		PHE A 3		29.978	32.949	28.245	1.00 27.31	A
	ATOM	1827	CD2	PHE A 3	301	29.560	31.050	26.845	1.00 27.89	A
	MOTA	1828	CE1	PHE A 3	301	31.205	32.403	28.625	1.00 28.83	A
	ATOM	1829	CE2	PHE A 3	301	30.781	30.498	27.217	1.00 28.05	A
30	ATOM	1830	CZ	PHE A 3		31.605	31.175	28.110	1.00 28.27	
	ATOM	1831	С	PHE A 3		26.459	34.384	25.619	1.00 28.27	· A
	ATOM	1832	ō	PHE A 3		25.946	35.261			A
	ATOM	1833	N	PRO A 3		25.798		26.317	1.00 32.36	A
	ATOM	1834	CD	PRO A 3		26.313	33.804	24.607	1.00 33.29	A
,35	ATOM	1835	CA	PRO A 3			32.943	23.529	1.00 34.04	A
,	ATOM	1836	CB	PRO A 3		24.415	34.199	24.341	1.00 35.24	•
	ATOM	1837	CG			24.144	33.608	22.959	1.00 34.01	Α
	ATOM	1838		PRO A 3		25.041	32.413	22.921	1.00 35.48	A
	ATOM		C	PRO A 3		23.567	33.561	25.444	1.00 37.39	A
40		1839	0	PRO A 3		23.935	32.518	25.986	1.00 38.49	Α
40	ATOM	1840	N	ALA A 3		22.447	34.188	25.783	1.00 39.36	A
	ATOM	1841	CA	ALA A 3		21.572	33.692	26.843	1.00 40.65	A
	ATOM	1842	CB	ALA A 3		20.280	34.506	26.862	1.00 41.66	A
	ATOM	1843	С	ALA A 3		21.238	32.197	26.814	1.00 41.25	A
	MOTA	1844	0	ALA A 3	03	21.253	31.537	27.854	1.00 43.16	· A
45	ATOM	1845	N	ALA A 3	04	20.945	31.665	25.631	1.00 41.04	A
	ATOM	1846	CA	ALA A 3	04	20.569	30.258	25.480	1.00 40.66	A
	ATOM	1847	CB	ALA A 3	04	20.121	30.004	24.040	1.00 41.36	A
	ATOM	1848	С	ALA A 3		21.628	29.223	25.876	1.00 39.61	A
	ATOM	1849	0	ALA A 3		21.298	28.156	26.395	1.00 39.01	
50	ATOM	1850		PHE A 3		22.891	29.543	25.617	1.00 36.21	A
	ATOM	1851		PHE A 3		24.022				A
	ATOM	1852		PHE A 3		25.259	28.662	25.909	1.00 32.08	A
	ATOM	1853		PHE A 30			29.519	26.187	1.00 29.46	A
	ATOM	1854				26.536	28.917	25.690	1.00 28.15	A
55	ATOM			PHE A 30		27.146	27.875	26.377	1.00 26.20	A
55		1855		PHE A 30		27.127	29.386	24.521	1.00 27.05°	A
	ATOM	1856		PHE A 30		28.330	27.308	25.908	1.00 26.92	Α
	ATOM	1857		PHE A 30		28.312	28.826	24.042	1.00 26.62	A
	ATOM	1858		PHE A 30		28.914	27.786	24.737	1.00 26.61	A
	ATOM	1859	С	PHE A 30)5	23.811	27.664	27.057	1.00 30.09	A

	ATOM	1860	0	PHE	A 305	23.518	28.051	28.187	1.00 31.51	75
	ATOM	1861	N		A 306	23.964		26.758	-,,,,,	. A
	ATOM	1862			A 306	23.801		27.769		A
	ATOM	1863	CB		A 306					A
5	ATOM	1864	CG		A 306	24.157		27.170	1.00 25.03	A
,						23.548		25.815	1.00 27.24	A
	ATOM	1865	CD.	1 PHE 2	4. 306	22.170		25.622	1.00 28.40	Α
	ATOM	1866	CD	PHE 2	306	24.350		24.728	1.00 27.84	A
	ATOM	1867		L PHE 2		21.601	23.603	24.365	1.00 28.05	A
	ATOM	1868		PHE A		23.792	23.155	23.465	1.00 28.31	A
10	ATOM	1869	cz		306	22.415	23.263	23.283	1.00 28.00	A
	ATOM	1870	С	PHE A	4.306	24.711	25.652	28.961	1.00 26.23	A
	ATOM	1871	0	PHE A	306	25.927	25.775	28.811	1.00 25.59	. A
	ATOM	1872	N		307	24.125		30.163	1.00 26.67	. A
	ATOM	1873	CD	PRO A		22.685		30.430	1.00 27.95	A
15	ATOM	1874	CA	PRO I		24.842		31.405	1.00 27.95	
	ATOM	1875	СВ	PRO F		23.795		32.481		A
	ATOM	1876	CG	PRO F					1.00 26.14	A
	ATOM	1877	C	PRO F		22.531		31.803	1.00 27.86	· A
	ATOM	1878				26.145		31.659	1.00 25.58	Α
20			0	PRO P		27.189		31.900	1.00 22.65	A
ຸ20	MOTA	1879	N	LYS F		26.085		31.620	1.00 24.46	А
	ATOM	1880	CA	LYS A		27.274		31.867	1.00 23.91	A
	ATOM	1881	СВ	LYS A		26.887		32.024	1.00 23.25	A
	MOTA	1882	CG	LYS A	308	26.062	21.532	33.285	1.00 28.49	A
	MOTA	1883	·CD	LYS A		25.618	20.093	33.466	1.00 30.17	A
25	ATOM	1884	CE	LYS A	308	24.760	19.973	34.722	1.00 33.12	A
	ATOM	1885	NZ	LYS A	308	24.122	18.636	34.860	1.00 34.13	A
	ATOM	1886	С	LYS A	308	28.314	23.426	30.769	1.00 22.84	A
	ATOM	1887	0	LYS A	308	29.514	23.411	31.042	1.00 22.46	, A
	MOTA	1888	N	ALA A	309	27.861	23.621	29.534	1.00 21.59	A
30	ATOM	1889	CÁ	ALA A		28.792	23.848	28.432	1.00 20.02	A
	ATOM	1890	СВ	ALA A		28.056	23.856	27.106	1.00 18.80	A
	ATOM	1891	C	ALA À		29.481	25.191	28.662	1.00 21.41	A
	ATOM	1892	Ö	ALA A		30.680	25.335	28.427	1.00 21.39	A
	ATOM	1893	N	ARG A		28.717	26.179	29.121	1.00 21.39	A
35	ATOM	1894	CA	ARG A		29.290	27.494	29.388		
33	ATOM	1895	CB	ARG A					1.00 22.02	. A
	ATOM	1896				28.213	28.479	29.854	1.00 22.39	A
			CG	ARG A		28.806	29.756	30.436	1.00 25.30	A
	ATOM	1897	CD	ARG A		27.780	30.852	30.664	1.00 28.33	A
40	ATOM	1898	NE	ARG A		28.420	32.039	31.230	1.00 30.18	A
40	ATOM	1899	CZ	ARG A		27.901	33.263	31.203	1.00 32.07	A
	ATOM	1900		ARG A		26.719	33.477	30.634	1.00 31.19	А
	MOTA	1901		ARG A		28.567	34.277	31.742	1.00 30.49	A
	ATOM	1902	С	ARG A		30.376	27.388	30.458	1.00 21.65	A
	ATOM	1903	0	ARG A		31.464	27.949	30.311	1.00 20.36	A
45	ATOM	1904	N	ASP A	311	30.074	26.677	31.541	1.00 19.57	A
•	MOTA	1905	CA	ASP A	311	31.043	26.512	32.615	1.00 20.18	Α
	ATOM	1906	CB	ASP A	311	30.460	25.649	33.739	1.00 20.39	A
•	ATOM	1907	CG	ASP A	311	31.439	25.446	34.881	1.00 23.35	A
	ATOM	1908	OD1	ASP A	311	32.158	24.428	34.885	1.00 24.91	A
50	ATOM	1909		ASP A		31.500	26.312	35.776	1.00 26.96	A
	ATOM	1910	C	ASP A		32.322	25.877	32.073	1.00 19.73	A
	ATOM	1911	ō	ASP A		33.422	26.289	32.439	1.00 19.30	A
	ATOM	1912	N	LEU A		32.179	24.891	31.188	1.00 15.30	A
	ATOM	1913	CA	LEU A		33.349	24.226	30.611		A
55	ATOM	1914	CB	LEU A		32.927			1.00 16.66	
55	ATOM	1914		LEU A			23.035	29.744	1.00 16.12	A
	ATOM		CG			34.050	22.320	28.974	1.00 14.73	A
		1916		LEU A		35.192	21.935	29.912	1.00 14.56	A
	MOTA	1917		LEU A		33.477	21.084	28.289	1.00 14.22	A
	ATOM	1918	· C	LEU A	312	34.181	25.189	29.774	1.00 16.61	A

-	ATOM	1919	0	LEU 2	A 312	35.402	25.241	29.910	1.00 16.20	А
	ATOM	1920	N		A 313	33.515	25.949	28.908	1.00 16.20	
	ATOM	1921	CA		A 313					A
	ATOM	1922				34.207	26.907	28.058	1.00 15.37	A
_			CB		A 313	33.216	27.648	27.130	1.00 16.42	A
5	ATOM	1923		VAL A		33.915	28.796	26.426	1.00 16.93	Α
	MOTA	1924	CG2	VAL A	A 313	32.644	26.672	26.103	1.00 17.88	A
	ATOM	1925	С	VAL A	A 313	34.960	27.923	28.911	1.00 17.39	A
	MOTA	1926	0	VAT. 7	313	36.093	28.294	28.591	1.00 18.00	
	ATOM	1927	N		A 314	34.342				A
10	ATOM	1928					28.364	30.004	1.00 17.61	A
10			CA	GLU A		34.986	29.331	30.885	1.00 20.43	A
	MOTA	1929	CB	GLU A		34.009	29.816	31.959	1.00 22.14	A
	ATOM	1930	CG	GLU A	A 314	32.800	30.550	31.396	1.00 26.52	A
	ATOM	1931	CD	GLU A		31.852	31.025	32.478	1.00 31.26	Α
	ATOM	1932	OE1	GLU A	314	31.580	30.246	33.417	1.00 33.48	A
15	ATOM	1933		GLU A		31.370	32.173	32.387	1.00 34.81	A
	ATOM	1934	C.	GLU A		36.217	28.721	31.539	1.00 19.15	A
	ATOM	1935	ō	GLU F						
						37.134	29.433	31.934	1.00 21.47	Α
	ATOM	1936	N	LYS F		36.245	27.400	31.651	1.00 19.51	A
	ATOM	1937	CA	LYS F		37.394	26.749	32.258	1.00 19.17	Α
20	ATOM	1938	CB	LYS A	315	36.946	25.514	33.043	1.00 18.84	A
	ATOM	1939	CG	LYS A	315	36.280	25.885	34.368	1.00 19.62	A
	ATOM	1940	CD	LYS A	315	35.653	24.696	35.073	1.00 19.22	A
•	ATOM	1941	CE	LYS A		35.070	25.095	36.427	1.00 21.00	A
	ATOM	1942	NZ	LYS A		36.119	25.552	37.381	1.00 19.53	
25	ATOM	1943	C	LYS A			26.393			A
23						38.452		31.218	1.00 18.96	A
•	MOTA	1944	0	LYS A		39.511	25.873	31.561	1.00 19.85	A
	MOTA	1945	N	LEU A		38.164	26.691	29.950	1.00 17.08	A
	ATOM	1946	CA	LEU A		39.102	26.429	28.854	1.00 16.41	Α
	ATOM	1947	CB	LEU A	316	38.414	25.636	27.738	1.00 13.81	A
30 -	ATOM	1948	CG	LEU A	316	38.028	24.201	28.115	1.00 14.39	A
	ATOM	1949	CD1	LEU A	316	37.139	23.597	27.031	1.00 12.38	A
	ATOM	1950		LEU A		39.302	23.373	28.309	1.00 12.77	Ä
	ATOM	1951	C	LEU A		39.652	27.743	28.290	1.00 17.12	A
	ATOM	1952	Ö	LEU A		40.851				
35		1953					27.860	28.023	1.00 16.53	
33	ATOM		N	LEU A		38.780	28.729	28.105	-	A
	ATOM	1954	CA	LEU A		39.228	30.022	27.596	1.00 17.52	A
	ATOM	1955	СВ	LEU A	. 317	38.083	30.752	26.887	1.00 16.37	A
	ATOM	1956	CG	LEU A	317	37.448	29.973	25.727	1.00 18.81	A
	ATOM	1957	CD1	LEU A	317	36.415	30.851	25.018	1.00 16.47	A
40	ATOM	1958	CD2	LEU A	317	38.528	29.526	24.741	1.00 17.87	A
	ATOM	1959	С	LEU A		39.745	30.841	28.774	1.00 18.27	A
	ATOM	1960	ō	LEU A			31.753	29.273	1.00 18.58	A
	ATOM	1961	N	VAL A		40.937	30.475	29.229	1.00 18.02	
	ATOM	1962								A
15			CA	VAL A		41.593	31.141	30.342	1.00 18.85	A
45	ATOM	1963		VAL A		41.846	30.153	31.500	1.00 19.91	А
	ATOM	1964		VAL A		42.590	30.848	32.634	1.00 20.01	Α
	ATOM	1965	CG2	VAL A	318	40.520	29.584	31.990	1.00 19.44	A
	ATOM	1966	C	VAL A	318	42.923	31.657	29.811	1.00 19.67	Α
	ATOM	1967	0	VAL A		43.690	30.902	29.208	1.00 18.26	A
50	ATOM	1968		LEU A		43.197	32.939	30.028	1.00 20.07	A
	ATOM	1969		LEU A		44.436	33.533	29.538	1.00 20.98	A
	ATOM	1970		LEU A		44.521				
							35.002	29.968	1.00 21.64	A
	ATOM	1971		LEU A		43.418	35.908	29.408	1.00 24.38	A
	ATOM	1972		LEU A		43.606	37.332	29.935	1.00 23.28	A
55	ATOM	1973		TEU Y		43.453	35.887	27.875	1.00 24.33	A
	ATOM	1974	С	LEU A	319	45.680	32.774	29.994	1.00 20.38	Α
	ATOM	1975		LEU A		46.568	32.496	29.192	1.00 21.34	A
	ATOM	1976		ASP A		45.742	32.440	31.280	1.00 20.22	A
	ATOM	1977		ASP A		46.879	31.707	31.833	1.00 20.90	A
							52.707	51.555		2.2

	ATOM	1978	CB	ASP A	320	46.842	31.760	33.365	1.00 20.76	A
	ATOM	1979	CG	ASP F		48.049	31.102	34.004		
	ATOM	1980		1 ASP F		48.669	30.226	33.367		A
	ATOM	1981		2 ASP A		48.371			1.00 23.46	A
5	ATOM	1982					31.450	35.159	1.00 23.89	A
,			C	ASP A		46.814	30.247	31.367	1.00 20.06	Α
	ATOM	1983	0	ASP A		45.988	29.476	31.840	1.00 20.54	A
	ATOM	1984	N	ALA A		47.700	29.876	30.451	1.00 20.68	Α
	ATOM	1985	CA	ALA A	321	47.733	28.522	29.903	1.00 22.04	A
	ATOM	1986	CB	ALA A	321	48.860	28.411	28.881	1.00 20.75	A
10	ATOM	1987	С	ALA A	321	47.858	27.400	30.940	1.00 21.62	A
	ATOM	1988	0	ALA A		47.482	26.259	30.665	1.00 21.02	. A
	ATOM	1989	N	THR A	_	48.372	27.715	32.127	1.00 20.89	
	ATOM	1990	·CA	THR A		48.531	26.698			A
	ATOM	1991	CB	THR A				33.167	1.00 20.82	A
15						49.670	27.051	34.146	1.00 19.47	A
13	ATOM	1992	OG1			49.341	28.253	34.848	1.00 20.19	A
	ATOM	1993	CG2			50.981	27.249	33.394	1.00 21.59	А
	ATOM	1994	. С	THR A		47.264	26.498	33.983	1.00 19.55	A
	ATOM	1995	Ο.	THR A	322	47.235	25.673	34.894	1.00 21.13	A
	MOTA	1996	N	LYS A	323	46.216	27.248	33.661	1.00 19.33	А
20	ATOM	1997	CA	LYS A	323	44.962	27.122	34.392	1.00 21.20	A
	ATOM	1998	СВ	LYS A	323	44.580	28.460	35.030	1.00 23.75	Α.
	ATOM	1999	CG	LYS A		45.562	28.933	36.084	1.00 28.45	A
	ATOM	2000	CD	LYS A		45.055	30.177	36.799	1.00 20.45	
	ATOM	2001	CE	LYS A		46.087				A
25	ATOM	2001	NZ	LYS A			30.678	37.802	1.00 36.15	A
23						46.532	29.569	38.693	1.00 37.34	A
		. 2003	C	LYS A		43.806	26.614	33.539	1.00 20.68	A
	ATOM	2004	0	LYS A		42.649	26.757	33.915	1.00 20.42	A
	MOTA	2005	N	ARG A		44.114	26.019	32.392	1.00 19.97	А
	ATOM	2006	CA	ARG A		43.060	25.494	31.531	1.00 17.98	A
30	ATOM	2007	CB	ARG A	324	43.461	25.609	30.061	1.00 15.95	A
	MOTA	2008	CG	ARG A	324	43.534	27.050	29.603	1.00 17.34	А
	ATOM	2009	CD	ARG A	324	43.996	27.194	28.172	1.00 19.80	Α
	ATOM	2010	NE	ARG A	324	44.438	28.565	27.944	1.00 16.93	A
	ATOM	2011	CZ	ARG A		45.410	28.908	27.108	1.00 19.88	A
35	ATOM	2012		ARG A		46.045	27.978	26.398	1.00 14.58	A
	ATOM	2013		ARG A		45.774	30.181	27.015	1.00 14.50	
	ATOM	2014	C	ARG A		42.762	24.046			. A
	ATOM	2015	Ö	ARG A				31.883	1.00 18.32	A
	ATOM					43.673	23.222	32.006	1.00 18.20	A
40		2016	N	LEU A	-	41.479	23.748	32.055	1.00 18.32	A
40	ATOM	2017	CA	LEU A		41.050	22.403	32.395	1.00 17.79	A
	ATOM	2018	CB	LEU A		39.523	22.335	32.425	1.00 17.03	A
	ATOM	2019	CG	LEU A		38.896	21.125	33.116	1.00 15.91	A
	ATOM	2020	CD1	LEU A	325	39.392	21.048	34.557	1.00 15.93	Α
	ATOM	2021	CD2	LEU A		37.375	21.255	33.084	1.00 16.56	A
45	ATOM	2022	С	LEU A	325	41.599	21.433	31.356	1.00 18.68	A
	ATOM	2023	0	LEU A	325	41.347	21.586	30.157	1.00 18.28	A
	ATOM	2024	N	GLY A	326	42.354	20.439	31.821	1.00 18.18	A
	ATOM	2025	CA	GLY A		42.931	19.462	30.915	1.00 16.36	A
	ATOM	2026	С	GLY A		44.443	19.558	30.807	1.00 10.30	A
50	ATOM	2027	Ö	GLY A		45.093	18.592			
	ATOM	2028	N					30.404	1.00 19.52	A
				CYS A		45.016	20.708	31.161	1.00 18.16	A
	ATOM	2029	CA	CYS A		46.463	20.867	31.075	1.00 19.30	A
	ATOM	2030	CB	CYS A		46.856	22.350	31.058	1.00 20.22	A
	ATOM	2031	SG	CYS A		46.782	23.200	32.649	1.00 21.97	A
55	ATOM	2032	С	CYS A		47.169	20.157	32.228	1.00 20.22	A
	ATOM	2033	0	CYS A	327	46.561	19.828	33.246	1.00 17.92	Α
	MOTA	2034	Ŋ	GLU A	328	48.463	19.933	32.053	1.00 20.51	A
	ATOM	2035	CA	GLU A		49.274	19.244	33.042	1.00 23.34	A
	ATOM	2036	CB	GLU A		50.710	19.139	32.507	1.00 28.68	A

	ATOM	2037	CC	CTII	220	.	754 10 26	7 21 176	1 00		_
			CG		328	50.7				38.24	A
	ATOM	2038	CD	GLU F		52.0				43.23	A
	ATOM	2039		GLU A		52.5				46.22	A
_	MOTA	2040		GLU A		52.6				44.90	A
5	ATOM	2041	· C	GLU A		49.2				22.11	A
	ATOM	2042	0	GLU A	328	49.1	19.16	1 35.437	1.00	20.27	Α
	ATOM	2043	N	GLU A	329	49.2	276 21.20	4 34.506	1.00	18.40	A
	ATOM	2044	CA	GLU A	329	49.2	248 21.87	5 35.801		20.13	A
	ATOM	2045	CB	GLU A	329	49.5				20.36	A
10	ATOM	2046	CG	GLU A		51.0		1 . 35.190		24.05	A
	ATOM	2047	CD	GLU A		51.1				25.93	A
	· ATOM	2048		GLU A		50.2				26.61	
	ATOM	2049		GLU A		52.3					A
	ATOM	2050								27.19	A
1.5			C	GLU A		47.8				19.36	Α
15	MOTA	2051	0	GLU A		47.7			1.00		A
	MOTA	2052	N	MET A		46.8			1.00	17.28	A
	ATOM	2053	CA	MET A		45.5				16.38	Α
	MOTA	2054	CB	MET A		44.4	74 21.833	35.294	1.00	17.65	A
	ATOM	2055	CG	MET A	330	44.4	60 23.365	35.311	1.00	22.95	Α
20	MOTA	2056	SD	MET A	330	44.1	86 24.026	36.979	1.00	26.78	A
	ATOM	2057	CE	MET A	330	42.4	35 23.712	2 37.186	1.00	24.69	A
	ATOM	2058	С	MET A	330	45.2	57 19.730		1.00		A
	ATOM	2059	0	MET A		44.1			1.00		A
	ATOM	2060	N	GLU A		46.3			1.00		A
25	ATOM	2061	CA	GLU A		46.2			1.00		A
23	ATOM	2062	CB	GLU A		45.6					
	ATOM	2063	CG	GLU A					1.00		A
						46.0			1.00		A
	MOTA	2064	CD	GLU A		47.5			1.00		A
20	ATOM	2065		GLU A		48.0			1.00		A
30	ATOM	2066		GLU A		48.3			1.00		A
	ATOM	2067	С	GLU A		45.6			1.00		A
	ATOM	2068	0	GLU A		45.1	07 15.602	35.636	1.00	20.40	A
	ATOM	2069	Ν.	GLY A	332	45.8	44 17.133	34.167	1.00	16.23	Α
	ATOM	2070	CA	GLY A	332	45.4	20 16.353	33.015	1.00	14.10	A
35	ATOM	2071	С	GLY A	332	43.9	82 16.154	32.596	1.00	13.54	A
	ATOM	2072	0	GLY A	332	43.0	63 16.864	33.017	1.00	11.96	· A
	ATOM	2073	N	TYR A	333	43.8			1.00		A
	ATOM	2074	CA	TYR A		42.5			1.00		A
	ATOM	2075	CB	TYR A		42.7			1.00		A
40	ATOM	2076	CG	TYR A		43.1			1.00		A
	ATOM	2077	CD1			42.2			1.00		A
	ATOM	2078	CE1			42.5					
		2079		TYR A					1.00		A
	ATOM					44.4			1.00		A
4	MOTA	2080		TYR A		44.8			1.00		A
45	ATOM	2081	CZ			43.9			1.00		A
	ATOM	2082	ОН	TYR A		44.2			1.00		Α
•	ATOM	2083	С	TYR A		41.4			1.00	15.23	A
	ATOM	2084	0	TYR A	333	40.2	78 14.323	31.846	1.00	16.63	Α
	MOTA	2085	N	GLY A	334	41.9	07 13.650	33.244	1.00	15.50	Α
50	ATOM	2086	CA	GLY A	334	40.9	57 13.100	34.202	1.00	15.07	A
•	ATOM	2087	С	GLY A	334	39.9	25 14.146		1.00	16.40	А
	ATOM	2088	0	GLY A		38.7			1.00		Α
	ATOM	2089	N	PRO A		40.3			1.00		A
	ATOM	2090	CD	PRO A		41.7			1.00		A
55	ATOM	2091	CA	PRO A		39.4			1.00		A
	ATOM	2092	CB	PRO A		40.3			1.00		A
	ATOM	2092	CG	PRO A					1.00		
						41.4					A
	ATOM	2094	C	PRO A		38.5			1.00		A
	MOTA	2095	0	PRO A	335	37.43	23 17.204	34.631	1.00	14.84	A

	ATOM ATOM	2096 2097	N CA	LEU A			39.184 38.450	16.971 17.465	33.257 32.094	1.00 16.12 1.00 15.52	. A A
		2098	CB	LEU A			39.396	17.653	30.898	1.00 13.32	A
	ATOM							17.000		1.00 14.39	A
_	ATOM	2099	CG	LEU A			38.770				
5	MOTA	2100		LEU A			37.836	19.182	29.662	1.00 11.25	A
	ATOM	2101		LEU A			39.884	18.285	28.528	1.00 14.11	A
	MOTA	2102	С	LEU A			37.321	16.508	31.714	1.00 16.28	A
	MOTA	2103	0	LEU A			36.176	16.921	31.540	1.00 15.51	A
	MOTA	2104	N	LYS A			37.640	15.225	31.592	1.00 17.22	A
10	MOTA	2105	CA	LYS A			36.624	14.243	31.235	1.00 17.39	A
	MOTA	2106	CB	LYS A	337		37.293	12.900	30.921	1.00 17.68	A
	MOTA	2107	CG	LYS A	337		38.170	12.994	29.676	1.00 22.31	A
	MOTA	2108	CD	LYS A	337		39.213	11.892	29.592	1.00 24.60	A
	ATOM	2109	CE	LYS A	337		38.620	10.560	29.189	1.00 24.76	Ą
15	ATOM	2110	NZ	LYS A	337		39.710	9.560	28.997	1.00 25.05	A
	ATOM	2111	С	LYS A			35.577	14.096	32.342	1.00 17.33	A
	ATOM	2112	0	LYS A			34.456	13.652	32.090	1.00 14.42	A
	ATOM	2113	N	ALA A			35.928	14.500	33.559	1.00 15.83	A
	ATOM	2114	CA	ALA A			34.989	14.395	34.674	1.00 17.52	A
20	ATOM	2115	СВ	ALA A			35.749	14.167	35.980	1.00 19.68	А
20	ATOM	2116	c	ALA A			34.095	15.621	34.804	1.00 18.83	Α
	ATOM	2117	Ö	ALA A			33.252	15.687	35.695	1.00 18.94	A
		2117	N	HIS A			34.262	16.596	33.918	1.00 19.42	A
	ATOM			HIS A			33.438	17.796	34.004	1.00 19.28	A
0.5	MOTA	2119	CA	HIS A			33.865	18.819	32.949	1.00 19.20	A
25	ATOM	2120	CB						33.074	1.00 13.20	A
	MOTA	2121	CG	HIS A			33.163	20.134	33.649	1.00 20.20	A
	ATOM	2122		HIS A			33.549	21.299		1.00 18.93	A
	ATOM	2123		HIS A			31.880	20.340	32.612		A
	ATOM	2124		HIS A			31.506	21.576	32.896	1.00 22.19	
30	MOTA	2125		HIS A			32.500	22.179	33.525	1.00 21.98	A
	ATOM	2126	С	HIS A			31.957	17.448	33.845	1.00 19.13	A
	MOTA	2127	0	HIS A			31.597	16.576	33.061	1.00 19.52	A
	ATOM	2128	N	PRO A			31.079	18.125	34.606	1.00 19.80	A
	ATOM	2129	CD	PRO A	340		31.424	19.119	35.640	1.00 19.08	A
35	MOTA	2130	CA	PRO A	340		29.630	17.900	34.569	1.00 20.52	A
	ATOM	2131	CB	PRO A	340		29.091	19.058	35.396	1.00 20.74	A
	ATOM	2132	CG.	PRO A	340		30.146	19.207	36.454	1.00 19.20	A
	ATOM	2133	C	PRO A	340		29.000	17.834	33.176	1.00 21.42	A
	MOTA	2134	0	PRO A	340		28.049	17.088	32.955	1.00 22.48	A
40	MOTA	2135	N	PHE A	341		29.528	18.606	32.237	1.00 21.33	A
	ATOM	2136	CA	PHE A	341		28.985	18.610	30.886	1.00 21.57	A
	ATOM	2137	CB	PHE A	341		29.739	19.624	30.017	1.00 21.64	A
	ATOM	2138	CG	PHE A	341		29.207	19.740	28.613	1.00 23.18	A
	ATOM	2139	CD1	PHE A	341		27.903	20.171	28.382	1.00 22.58	Α
45	ATOM	2140		PHE A			30.013	19.431	27.522	1.00 21.95	A
	ATOM	2141		PHE A			27.410	20.292	27.082	1.00 23.54	A
	ATOM	2142		PHE A			29.533	19.548	26.220	1.00 21.83	A
	ATOM	2143	CZ	PHE A			28.228	19.980	25.998	1.00 23.23	Α
	ATOM	2144	C	PHE A		•	29.055	17.226	30.237	1.00 21.84	Α
50	ATOM	2145	Ö	PHE A			28.232	16.896	29.389	1.00 20.37	A
30	MOTA	2146		PHE A			30.034	16.422	30.640	1.00 20.51	A
			N	PHE A			30.221	15.085	30.077	1.00 23.01	A
	ATOM	2147	CA	PHE A			31.710	14.809	29.850	1.00 18.00	A
	ATOM	2148	CB					15.812	28.971	1.00 17.05	A
	ATOM	2149	CG	PHE A			32.398 32.010		27.652	1.00 17.03	A
55	MOTA	2150		PHE A				15.987	29.450	1.00 17.70	A
	ATOM	2151	-	PHE A			33.487	16.534	26.811	1.00 13.72	Ā
	MOTA	2152		PHE A			32.702	16.867			A
	MOTA	2153		PHE A			34.184	17.414	28.617	1.00 17.45	A
	ATOM	2154	CZ	PHE. A	342		33.790	17.578	27.298	1.00 16.56	A

								•				
	MOTA	2155	С	PHE	A	342	29.679	13.972	30.976	1.00	24.95	A
	ATOM	2156	0	PHE	Α	342	30.002	12.798	30.777	1.00	23.95	A
	ATOM	2157	N	GLU	A	343	28.861	14.333	31.958	1.00	27.35	Α
	MOTA	2158	CA	GLU	Α	343	28.325	13.349	32.897	1.00	30.28	А
5	ATOM	2159	CB.	GLU	Α	343	27.187	13.964	33.716	1.00	32.20	A
	ATOM	2160	CG	GLU			26.581	12.991	34.714	1.00	39.71	A
	ATOM	2161	CD	GLU			25.628	13.661	35.688		44.72	A
	ATOM	2162		GLU			24.661	14.314	35.234		47.55	A
	ATOM	2163		GLU			25.847	13.526	36.911		46.89	A
10	ATOM	2164	C	GLU			27.852	12.017	32.305		28.98	A
10	ATOM	2165	Ö	GLU			28.225	10.952	32.800		31.73	A
	ATOM	2166	N ·	SER			27.037	12.067	31.258		26.09	A
		2167	CA	SER			26.520	10.838	30.656		28.36	A
	ATOM	2168					25.129	11.089	30.067		28.73	A
15	ATOM		CB	SER					28.940		30.91	A
15	ATOM	2169	OG	SER			25.203	11.942	29.577		27.66	A
	ATOM	2170	C	SER			27.407	10.214				
	ATOM	2171	0	SER			26.987	9.281	28.900		28.66	A
	ATOM	2172	N			345	28.627	10.715	29.419		.26.75	A
	MOTA	2173	CA	VAL			29.534	10.183	28.402		23.44	A
20	ATOM	2174	CB	VAL			30.565	11.256	27.950		23.10	A
	MOTA	2175		VAL	-		31.589	10.631	26.995		22.24	A
	ATOM	2176		VAL			29.854	12.418	27.275		20.05	A
	MOTA	2177	C	VAL			30.326	8.957	28.855		24.26	A
	MOTA	2178	0	VAL			30.876	8.930	29.960		22.83	A
25	MOTA	2179	N	THR			30.374	7.942	27.997		21.77	A
	MOTA	2180	CA	THR			31.153	6.740	28.272		23.70	A
	ATOM	2181	CB	THR	Α	346	30.391	5.455	27.857		26.53	Α
	ATOM	2182		THR			29.248	5.284	28.706		29.98	A
	ATOM	2183	CG2	THR	A	346	31.289	4.231	27.990		24.28	A
30	MOTA	2184	С	THR	A	346	32.383	6.945	27.385		23.43	A
•	ATOM	2185	0	THR	Α	346	32.306	6.827	26.160		24.50	A
	ATOM ·	2186	N	TRP	Α	347	33.508	7.270	28.013		22.98	A
	MOTA	2187	CA	TRP	Α	347	34.744	7.569	27.300		23.81	A
	ATOM	2188	CB	TRP	Α	347	35.683	8.352	28.219	1.00	22.54	A
35	ATOM	2189	CG	TRP	Α	347	35.128	9.658	28.693		20.61	A
	ATOM	2190	CD2	TRP	Α	347	35.257	10.927	28.040	1.00	19.11	· A
	ATOM	2191	CE2	TRP	Α	347	34.581	11.881	28.838	1.00	18.39	Α
	ATOM	2192	CE3	TRP	Α	347	35.878	11.351	26.858	1.00	18.16	Α
	ATÓM	2193	CD1	TRP	Α	347	34.397	9.883	29.828	1.00	18.35	· A
40	ATOM	2194	NE1	TRP	Α	347	34.065	11.218	29.923	1.00	19.51	Α
	ATOM	2195	CZ2	TRP	Α	347	34.510	13.234	28.491	1.00	16.88	A
	ATOM	2196	CZ3	TRP	Α	347	35.808	12.701	26.511	1.00	17.23	Α
	ATOM	2197	CH2	TRP	Α	347	35.127	13.624	27.327	1.00	18.16	A
	ATOM	2198	С	TRP			35.538	6.429	26.675	1.00	25.79	Α
45	ATOM	2199	0	TRP			36.304	6.654	25.742	1.00	24.67	A
	ATOM	2200	N	ALA			35.360	5.215	27.183		27.10	Α
	ATOM	2201	CA	ALA			36.116	4.063	26.697		27.46	A
	ATOM	2202	CB	ALA			35.899	2.869	27.636		27.09	А
	ATOM	2203	C	ALA			35.895	3.620	25.256		27.18	А
50	ATOM	2204	Ö	ALA			36.830	3.148	24.613		29.41	A
50	ATOM	2205	N	ASN			34.682	3.769	24.735		26.55	A
	ATOM	2206	CA	ASN			34.418	3.310	23.375		27.28	A
	ATOM	2207	CB	ASN			33.700	1.962	23.444		29.37	A
	ATOM	2207	CG	ASN			32.299	2.088	24.013		30.92	A
55	ATOM	2209		ASN			32.045	2.942	24.859		30.17	A
,,	ATOM	2210		ASN			31.386	1.237	23.553		33.52	A
	ATOM			ASN			33.599	4.265	22.509		26.47	A
		2211 2212	C	ASN			32.669	3.843	21.819		25.87	A
	ATOM		0					5.543	22.518		24.45	A
	ATOM	2213	N	LEU	M	220	33.947	5.545	22.010.	1.00	- 4.45	1-1

	ATOM	2214	CĄ	LEU			33.203	6.510	21.721	1.00 23.14	
	MOTA	2215	CB	LEU	A	350	33.837	7.898	21.848	1.00 23.22	2 A
	ATOM	2216	CG	LEU	A	350	33.659	8.605	23.191	1.00 21.05	5 A
	ATOM	2217	CD1	LEU	Α	350	34.646	, 9.756	23.293	1.00 19.30	5 A
5	ATOM	2218	CD2	LEU	A	350	32.220	9.094	23.319	1.00 18.78	3 A
	ATOM	2219	С	LEU	Α	350	33.082	6.152	20.240	1.00 22.60) A
	ATOM	2220	0	LEU	Α	350	32.011	6.296	19.650	1.00 21.15	5 A
	ATOM	2221	N	HIS	Α	351	34.165	5.689	19.627	1.00 23.13	3 A
	ATOM	2222	CA	HIS	Α	351	34.089	5.387	18.204	1.00 27.83	3 A
10	ATOM	2223	СВ	HIS	Α	351	35.506	5.325	17.596	1.00 29.36	6 A
	ATOM	2224	CG	HIS			36.082	3.950	17.493	1.00 32.07	7 A
	ATOM	2225		HIS			36.611	3.128	18.431	1.00 32.39	
	MOTA	2226		HIS			36.197	3.285	16.291	1.00 33.02	
	ATOM	2227		HIS			36.775	2.113	16.493	1.00 33.58	
15	ATOM	2228		HIS			37.036	1.992	17.782	1.00 31.76	
1,3	MOTA	2229	C	HIS			33.258	4.144	17.874	1.00 28.12	
	ATOM	2230	Ö	HIS			33.015	3.847	16.707	1.00 29.49	
	ATOM	2231	N	GLN			32.800	3.442	18.908	1.00 29.28	
		2231		GLN			31.963	2.255	18.726	1.00 29.67	
20	MOTA	2232	CA	GLN			32.366		19.694	1.00 30.56	
20	ATOM		CB	GLN			33.169	0.041	19.034	1.00 30.88	
	ATOM	2234	CG	GLN				-0.186	19.729	1.00 30.00	
	MOTA	2235	CD				34.493	-0.150	20.928	1.00 31.23	•
	ATOM	2236		GLN			34.541		18.971	1.00 30.70	
0.5	ATOM	2237		GLN			35.578	-0.084		1.00 32.30	
25	ATOM	2238	С	GLN			30.504	2.638	18.963		
	MOTA	2239	0	GLN			29.595	1.831	18.770	1.00 29.01	
	ATOM	2240	N .	GLN			30.290	3.875`	19.397	1.00 27.64	
	MOTA	2241	CA	GLN			28.948	4.365	19.652	1.00 27.42	
	MOTA	2242	СВ	GLN			28.977	5.401	20.775		
30	MOTA	2243	CG	GLN			29.408	4.837	22.115	1.00 27.34	
	ATOM	2244	CD	GLN			29.638	5.914	23.156	1.00 27.19	
	MOTA	2245		GLN			28.875	6.872	23.252	1.00 28.29	
	MOTA	2246		GLN			30.687	5.753	23.951	1.00 28.79	
	ATOM	2247	С	GLN			28.375	4.989	18.385	1.00 29.00	
35	MOTA	2248	0	ĢLN			29.118	5.455	17.516	1.00 29.14	
	ATOM	2249	N	THR			27.053	4.984	18.276	1.00 27.3	
	ATOM	2250	CA	THR			26.390	5.568	17.119	1.00 27.85	
	ATOM	2251	СВ	THR			24.991	4.941	16.904	1.00 30.69	
	MOTA	2252		THR			25.132	3.532	16.665	1.00 30.0	
40	ATOM	2253		THR		•	24.289	5.585	15.709	1.00 29.58	
	ATOM	2254 .	С	THR			26.244	7.062	17.376	1.00 26.85	
	ATOM	2255	0	THR	A	354	25.592	7.475	18.329	1.00 25.77	
	MOTA	2256	N	PRO			26.867	7.898	16.533	1.00 27.22	
	ATOM	2257	CD	PRO	A	355	27.792	7.588	15.431	1.00 25.89	
45	ATOM	2258	CA	PRO			26.763	9.346	16.734	1.00 27.23	
	ATOM	2259	CB	PRO	Α	355	27.625	9.915	15.609	1.00 24.93	
	ATOM	2260	CG	PRO			28.643	8.838	15.385	1.00 25.54	
	ATOM	2261	С	PRO	Α	355	25.322	9.837	16.641	1.00 28.0	
	ATOM	2262	0	PRO	A	355	24.548	9.364	15.810	1.00 27.24	
50	MOTA	2263	N	PRO	Α	356	24.941	10.792	17.500	1.00 28.28	3 A
	MOTA	2264	CD	PRO	Α	356	25.752	11.560	18.462	1.00 28.33	
	ATOM	2265	CA	PRO	Α	356	23.572	11.306	17.448	1.00 28.4	1 A
	ATOM	2266	СВ	PRO -			23.539	12.301	18.604	1.00 28.13	
	ATOM	2267	CG	PRO			24.946	12.832	18.612	1.00 26.86	5 A
55	MOTA	2268	C	PRO			23.363		16.097	1.00 29.25	5 A
	ATOM	2269	Ō	PRO			24.304	12.537	15.529	1.00 27.27	
	ATOM .		N	ALA			22.143	11.910	15.575	1.00 30.45	
	ATOM	2271	CA	ALA			21.848	12.521	14.287	1.00 32.83	
	ATOM	2272	CB	ALA			20.507	12.019	13.757	1.00 31.99	
		. –	_		-						

	ATOM	2273	С	ALA	Α	357	21.824	14.035	14.448	1.00 35.05	A
	ATOM	2274	Ō	ALA	Α	357	21.194	14.561	15.369	1.00 35.04	A
	ATOM	2275	N	LEU	Α	358	22.516	14.730	13.552	1.00 37.81	A
	ATOM	2276	CA	LEU	Α	358	22.578	16.185	13.597	1.00 42.15	A
5	ATOM	2277	СВ	LEU	Α	358	23.679	16.681	12.658	1.00 39.54	A
_	ATOM	2278	CG			358	25.086	16.285	13.109	1.00 39.51	A
·	ATOM	2279		LEU			26.102	16.686	12.062	1.00 39.29	A
	MOTA	2280		LEU			25.395	16.953	14.445	1.00 40.01	A
	ATOM	2281	C			358	21.241	16.837	13.242	1.00 45.91	· A
10	ATOM	2282	ō			358	20.874	16.927	12.069	1.00 45.71	A
•	ATOM	2283	N	THR			20.530	17.290	14.275	1.00 50.06	A
	ATOM	2284	CA			359	19.223	17.939	14.140	1.00 53.73	A
	ATOM	2285	CB	THR			19.353	19.428	13.726	1.00 54.04	A
	ATOM	2286	OG1				19.995	19.521	12.448	1.00 56.35	A
15	ATOM	2287		THR			20.158	20.204	14.763	1.00 54.32	A
	ATOM	2288	C.	THR			18.309	17.236	13.139	1.00 54.47	A
	ATOM	2289	0	THR			18.483	16.016	12.930	1.00 55.90	A
	ATOM	2290		THR			17.407	17.908	12.595	1.00 56.97	A
	ATOM	2291	OH2	TIP	s	1	42.566	19.118	34.302	1.00 30.57	S
20	ATOM	2292	OH2		s	2	41.052	32.378	19.857	1.00 15.82	S
20	ATOM	2293	OH2		s	3	37.014	33.030	17.747	1.00 16.95	S
	ATOM	2294	OH2		s	5	45.353	24.370	18.152	1.00 16.85	S
	ATOM	2295	OH2		s	6	31.896	13.930	33.235	1.00 20.42	S
	ATOM	2296	OH2		s	7	50.351	22.781	28.249	1.00 20.42	S
25	ATOM	2297	OH2		s	8	45.246	-0.589	-0.734	1.00 17.74	S
	ATOM	2298		TIP	s	11	46.249	-0.348	-8.523	1.00 21.32	S
	ATOM	2299	OH2		s	14	45.756	11.148	29.680	1.00 21.94	S
	ATOM	2300	OH2		s	15	44.273	13.157	34.592	1.00 15.61	s
	ATOM	2301	OH2	TIP	S	17	53.598	3.722	-1.720	1.00 21.45	
30	ATOM	2302	OH2		S	18	46.049	13.087	31.565	1.00 20.35	s
	ATOM	2303	OH2		s	19	53.422	22.401	-3.280	1.00 23.26	S
	MOTA	2304	OH2	TIP	s	20	34.587	7.922	5.383	1.00 22.58	S
	ATOM	2305	OH2	TIP	s	21	45.053	27.379	19.376	1.00 29.60	S
	ATOM	2306	OH2	TIP	s	23	28.899	36.416	28.633	1.00 31.68	s
35	ATOM	2307	OH2	TIP	s	24	35.531	11.645	-8.219	1.00 23.45	S
	ATOM	2308	OH2	TIP	s	25	47.364	28.787	19.612	1.00 23.03	S
	ATOM	2309	OH2	ŢIP	S	27	48.859	21.588	12.634	1.00 23.76	·S
	ATOM	2310	OH2	TIP	S	29	48.805	8.920	23.626	1.00 22.23	S
	ATOM	2311	OH2	TIP	S	31	48.619	7.247	10.112	1.00 21.32	s
40	ATOM	2312	OH2	TIP	S	34	44.824	28.720	15.621	1.00 25.27	s
	ATOM	2313	OH2		S	35	26.030	12.634	13.407	1.00 21.61	S
	ATOM	2314	OH2	TIP	S	36	50.462	19.810	40.066	1.00 25.45	S
	ATOM	2315	OH2		S	37	39.631	23.510	-0.239	1.00 30.88	S
	ATOM	2316	OH2		S	40	44.734	42.655	10.346	1.00 30.84	S
45	ATOM	2317		TIP		41	54.653	3.902	1.503	1.00 27.14	S
	ATOM	2318		TIP		45	45.693	21.923	39.754	1.00 28.30	S
	ATOM	2319		TIP		47	47.820	16.413	7.805	1.00 25.73	S
	ATOM	2320		TIP		48	50.292	31.412	29.642	1.00 32.79	S
	ATOM	2321		TIP		49	26.056	16.646	34.827	1.00 29.80	s
50	ATOM	2322		TIP		52	31.714	10.996	31.855	1.00 29.15	S
	ATOM	2323		TIP		53	46.108	23.843	-4.299	1.00 24.21	S
	ATOM	2324		TIP		54	37.645	11.206	34.448	1.00 28.56	S
	ATOM	2325		TIP		55	26.371	28.513	12.142	1.00 32.08	S
	ATOM	2326.		TIP		58	33.564	19.700	3.483	1.00 28.28	S
55	ATOM	2327		TIP		64	48.295	-0.632	14.280	1.00 32.13	S
	ATOM	2328		TIP		65	40.064	26.036	34.324	1.00 24.17	S
	ATOM	2329		TIP		66	29.570	3.958	14.729	1.00 28.94	S
	ATOM	2330		TIP		72	60.085	11.604	6.814	1.00 38.35	S
	ATOM	2331	OH2	TIP	S	73	39.203	44.403	18.686	1.00 26.61	S

	ATOM	2332	OH2 TIP S	76	47.312	12.366	27.366	1 00	28.51	
		2333					_			S
	ATOM		OH2 TIP S			33.771			28.82	S.
	ATOM	2334	OH2 TIP S	81	57.890	13.106	2.128	1.00	40.62	S
	ATOM	2335	OH2 TIP S	82	41.663	34.381	32.043	1.00	19.35	s
5	MOTA	2336	OH2 TIP S		50.974	40.331			21.14	s
•	ATOM	2337	OH2 TIP S		47.925	-0.832				
									24.11	. S
	ATOM	2338	OH2 TIP S		27.231	28.336			27.64	S
	MOTA	2339	OH2 TIP S	91	43.651	-7.101	-7.995	1.00	24.33	S
	MOTA	2340	OH2 TIP S	92	49.325	4.387	19.370	1.00	28.02	s
10	ATOM	2341	OH2 TIP S	93	46.231	11.549	33.898		29.40	S
	ATOM	2342	OH2 TIP S		63.889	24.831	1.168		26.53	S
	MOTA	2343		-	56.396	4.952	-6.749		28.00	S
	MOTA	2344	OH2 TIP S		35.510	27.986			29.24	s
	MOTA	2345	OH2 TIP S	100	49.942	24.366	30.265	1.00	31.61	S
15	MOTA	2346	OH2 TIP S	101	56.121	7.113	-8.298	1.00	31.57	S
	ATOM	2347	OH2 TIP S		58.318	19.957	-8.378		26.95	S
	ATOM	2348	OH2 TIP S		49.647	22.446	39.624		40.57	
										S
	ATOM	2349	OH2 TIP S		45.359	7.052	13.052		26.27	S
	MOTA	2350	OH2 TIP S		37.150	32.340	32.346	1.00	34.45	S
20	MOTA	2351	OH2 TIP S	107	43.465	40.457	8.240	1.00	40.48	S
	ATOM	2352	OH2 TIP S	119	36.644	8.257	13.418	1.00	30.70	s
	ATOM	2353		123	41.912	-8.974	-8.264		26.08	s
	ATOM	2354	OH2 TIP S							
					62.424	15.800	-7.411			S
	ATOM	2355	OH2 TIP S		37.266	18.656	-9.097		28.99	_. S
25	MOTA	2356	OH2 TIP S	127	43.129	26.845	14.606	1.00	25.19	· s
	ATOM	2357	OH2 TIP S	128	36.339	32.639	29.802	1.00	29.25	S
	MOTA	2358	OH2 TIP S	130	54.051	14.561	26.498	1.00	33.93	s
	ATOM	2359	OH2 TIP S		41.805	-4.242	5.492		33.72	s
	ATOM	2360	OH2 TIP S		38.873	25.163	36.697		30.69	S
20										
30	MOTA	2361	OH2 TIP S		28.777	8.553	25.307		31.43	S
	ATOM	2362	OH2 TIP S		53.672	10.546	-12.803	1.00	33.45	S
	ATOM	2363	OH2 TIP S	136	59.892	15.434	11.467	1.00	31.39	S
	MOTA	2364	OH2 TIP S	137	31.040	12.361	35.470	1.00	34.07	S
	ATOM	2365	OH2 TIP'S		33.489	14.292	-0.598		40.68	S
35	ATOM	2366	OH2 TIP S		46.918	8.748	11.662		29.23	s
55										
	ATOM	2367	OH2 TIP S		46.297	-7.287	-9.196		42.20	S
	MOTA	2368	OH2 TIP S		58.193	6.715	-4.685		35.48	s.
	ATOM	2369	OH2 TIP S	143	44.598	4.435	12.503	1.00	27.68	s
	MOTA	2370	OH2 TIP S	144	27.003	5.999	12.450	1.00	36.30	S
40	ATOM	2371	OH2 TIP S	145	43.676	32.852	35.735	1.00	35.70	S
	ATOM	2372	OH2 TIP S	146	35.783	18.628	36.452		34.62	s
	ATOM	2373	OH2 TIP S		25.402				45.03	s
						4.058	20.638			
	ATOM	2374	OH2 TIP S	148	45.839	35.853	33.724		35.47	S
	MOTA	2375	OH2 TIP S		22.176	18.976	16.752	1.00	31.87	S
45	ATOM	2376	OH2 TIP S	150	43.986	33.179	10.162	1.00	37.70	s
	ATOM	2377	OH2 TIP S	151	50. <i>6</i> 53	20.347	42.428	1.00	35.80	s
	ATOM	2378	OH2 TIP S		47.843	24.314	9.506		31.05	S
	ATOM	2379	OH2 TIP S		44.693				29.90	S
							-14.175			
	ATOM	2380	OH2 TIP S		26.560	36.851	31.684		49.29	S
50	MOTA	2381	OH2 TIP, S		46.867	8.019	-12.951	1.00	29.21	S
	ATOM	2382	OH2 TIP S	157	30.432	28.741	12.438	1.00	37.76	s
	ATOM	2383	OH2 TIP S	158	41.004	20.553	6.423	1.00	39.53	S
	ATOM	2384	OH2 TIP S		49.258	20.069	29.294		33.97	S
	ATOM	2385	OH2 TIP S		48.082	28.459				s
5.5							16.489		33.10	
55	ATOM	2386	OH2 TIP S		47.448	18.625	27.683		34.87	S
	ATOM	2387	OH2 TIP S		19.687	20.632	23.411		35.01	S
	ATOM	2388	OH2 TIP S	163	32.402	-1.266	22.443		37.26	s
	ATOM	2389	OH2 TIP S	164	39.475	33.468	33.237	1.00	35.34	S
	ATOM	2390	OH2 TIP S		44.277	18.950	5.162	1.00		s
										-

	ATOM	2391	OH2 TIP S	166	34.797	30.523	10.736	1.00 47.55	S
	ATOM	2392	OH2 TIP S	167	46.541	3 526	-14.949	1.00 26.54	·S
	ATOM	2393	OH2 TIP S		36.333			1.00 38.68	
									S
	ATOM	2394	OH2 TIP S		•			1.00 34.66	S
5	ATOM	2395	OH2 TIP S	170	24.163	13.264	11.375	1.00 41.23	S
	ATOM	2396	OH2 TIP S	171	48.459		31.951	1.00 38.11	S
	ATOM	2397	OH2 TIP S		34.261				
								1.00 48.96	S
	MOTA	2398		173	45.924	-0.026	13.224	1.00 39.55	S
	ATOM	2399	OH2 TIP S	175	41.384	37.389	32.543	1.00 40.74	S
10	ATOM	2400	OH2 TIP S	177	49.394	35.312	27.150	1.00 44.33	, s
	ATOM	2401	OH2 TIP S		29.066			1.00 41.46	
									S
	MOTA	2402	OH2 TIP S		49.354	19.467	7.273	1.00 34.56	s
	ATOM	2403	OH2 TIP S	181	25.298	17.029	31.863	1.00 47.74	S
	ATOM	2404	OH2 TIP S	182	37.071	25.027	4.669	1.00 43.87	s
15	ATOM	2405	OH2 TIP S		22.581		18.691		S
13								1.00 41.75	
	MOTA	2406	OH2 TIP S		32.269		-1.891	1.00 48.84	S
	ATOM	2407	OH2 TIP S	185	48.234	0.494	6.833	1.00 48.16	S
	ATOM	2408	OH2 TIP S	187	. 20.008		19.211	1.00 45.27	s
	ATOM	2409	OH2 TIP S		49.341		42.272	1.00 42.20	S
00									
20	ATOM	2410	OH2 TIP S		61.292	18.260	-8.097	1.00 45.21	s
	ATOM	2411	OH2 TIP S	191	28.152	10.606	2.819	1.00 40.38	S
	ATOM	2412	OH2 TIP S	192	25.626	12.619	23.191	1.00 34.27	s
	ATOM	2413	OH2 TIP S		59.876		1.216	1.00 46.54	S
	ATOM	2414		194	57.592		-10.646	1.00 45.82	S
25	ATOM	2415	OH2 TIP S	195	31.509	36.649	21.499	1.00 38.73	S
	ATOM	2416	OH2 TIP S	197	50.270	-1.543	-6.136	1.00 42.66	S
	ATOM	2417	OH2 TIP S	198	24.467	8.729	13.088	1.00 42.78	S
			OH2 TIP S					1.00 32.80	
	ATOM	2418			38.098	8.699			S
	MOTA	2419	OH2 TIP S	200	57.831	11.358	-13.255	1.00 45.31	. S
30	ATOM	2420	OH2 TIP S	201	23.888	22.328	30.524	1.00 37.12	Š
	ATOM	2421	OH2 TIP S	202	47.691	26.068	37.666	1.00 37.92	s
	ATOM	2422	OH2 TIP S		38.653	7.070	29.307	1.00 50.54	S
	ATOM	2423			44.424	27.583	2.092	1.00 53.50	S
	ATOM	2424	OH2 TIP S	212	22.258	2.296	17.948	1.00 47.38	S
35	ATOM	2425	OH2 TIP S	214	19.843	17.943	23.303	1.00 30.36	S
	ATOM	2426			27.647	11.344	24.681	1.00 31.32	Ş
		2427							S
	ATOM		OH2 TIP S	217	37.953	7.817	-9.284	1.00 45.97	
	ATOM	2428	OH2 TIP S		33.845	34.040	12.124	1.00 38.11	S
	ATOM	2429	OH2 TIP S	219	58.484	15.269	13.717	1.00 38.26	S
40	ATOM	2430	OH2 TIP S	220	48.526	40.920	26.583	1.00 35.23	s
	ATOM	2431	OH2 TIP S		52.094	21.184	38.122	1.00 29.86	s
	ATOM	2432		223	36.889	5.881	3.281	1.00 37.63	S
	MOTA	2433	OH2 TIP S	224	47.642	-1.401	-10.684	1.00 34.89	S
	ATOM	2434	OH2 TIP S	226	47.284	2.916	19.133	1.00 34.10	S
45	ATOM	2435	OH2 TIP S	227	42.468	4-463	-15.039	1.00 37.98	s
	ATOM	2436	OH2 TIP S		19.169		21.831	1.00 41.57	S
	MOTA	2437	OH2 TIP S		57.592	12.689		1.00 50.22	S
	MOTA	2438	OH2 TIP S	232	27.102	9.176	5.655	1.00 40.57	S
	ATOM	2439	OH2 TIP S	233	58.618	9.072	-11.925	1.00 50.71	· s
50	ATOM	2440	OH2 TIP S		22.822	25.342	19.945	1.00 34.93	S
50									
	MOTA	2441	OH2 TIP S		24.831	32.218	28.901	1.00 37.69	S
	ATOM	2442	OH2 TIP S		20.045	10.774	16.992	1.00 39.57	S
	ATOM	2443	OH2 TIP S	238	58.019	19.850	15.679	1.00 41.42	S
	ATOM	2444	OH2 TIP S		19.490	20.949	26.114	1.00 34.55	S
55	ATOM	2445	OH2 TIP S		61.187	26.377	7.346	1.00 39.68	Ş
J.J									
	ATOM	2446	OH2 TIP S		33.680	38.342	19.389	1.00 48.93	S
	ATOM	2447	OH2 TIP S	242	51.539	31.612	10.881	1.00 55.65	S
	ATOM	2448	OH2 TIP S	244	25.872	14.431	30.404	1.00 46.69	S
	ATOM	2449	OH2 TIP S		37.332	5.849	9.544	1.00 43.81	S
	111011	2277	7115 TTT D	230	31.332	3.049	2.277	2.00 40.01	J

	ATOM	2450	0113	TTD	S 25	Λ.		39.087	-1.293	-9.655	1 00	42.96		S
	•													
	ATOM	2451			S 25			23.938	30.000	30.010		38.89		S
	MOTA	2452			S 25			24.949	29.749	32.578	1.00	40.17		S
	MOTA	2453	OH2	TIP	S 26	0		32.111	17.986	1.918	1.00	48.36		s
5	ATOM	2454	OH2	TIP	S 26	6		21.404	12.876	25.603	1.00	57.17		S
	ATOM	2455	OH2	TIP	S 26	9		35.425	36.767	12.550	1.00	30.70		S
	ATOM	2456	OH2					52.438	25.529	30.131		44.85		s
							-		20.156	36.003				
	MOTA	2457	OH2		S 27			53.299				37.15		s
	ATOM	2458			S 27			50.914	6.919	23.723		43.29		s
10	MOTA	2459	OH2		S 27	4		31.578	30.795	11.014	1.00	50.15		S
	ATOM	2460	OH2	TIP	S 27	5		26.341	7.243	22.447	1.00	39.40		S
	MOTA	2461	OH2	TIP	s 27	6		60.392	18.195	10.235	1.00	37.91		S
	ATOM	2462	OH2					47.355		-10.821		48.18		S
	ATOM	2463	OH2		S 27			41.304		-16.647		38.12		s
1.5														S
15	MOTA	2464		TIP				33.299	21.620	37.881		46.29		
	MOTA	2465		TIP				56.469	26.112	-8.575		43.71		S
	ATOM	2466	OH2	TIP	S 28	7		48.382	26.573	7.246	1.00	41.43		S
	ATOM	2467	OH2	TIP	S 28	8		56.240	7.245	-11.331	1.00	41.79		S
	ATOM	2468	OH2	TIP	S 29	0		49.060	14.978	28.166	1.00	37.03		s
20	ATOM	2469	OH2		S 29			37.095	44.270	26.442	1.00	45.08	•	S
20	ATOM	2470		TIP				47.814		-13.299		48.60		s
		2471	OH2		S 29			58.081	2.784	-7.841		41.89		s
	MOTA											54.91		s
	MOTA	2472	OH2		S 29			36.447	45.321	18.644				
	ATOM	2473	OH2		S 29			49.029	23.328	1.767		30.55		S
25	MOTA	2474	OH2					24.375	13.771	8.634		48.47		S
	ATOM	2475	OH2	TIP	S 30	3		47.904	36.798	28.653	1.00	35.76		S
٠.	ATOM	2476	OH2	TIP	S 30	5		51.156	40.821	27.172	1.00	43.59		S
	ATOM	2477	OH2	TIP	S 30	6		32.943	28.917	35.227	1.00	42.60		s
	ATOM	2478	OH2	TIP	s 30	7		58.462	28.373	6.251	1.00	46.15		s
30	ATOM	2479		TIP				41.964	30.940	36.712	1.00	48.26		S
50		2480	OH2		s 31			51.176	-1.922	-3.336		50.61		S
	ATOM		OH2		\$100			21.319	36.868	23.805		36.97		s
	ATOM	2481								27.617		44.40		s
	ATOM	2482	OH2		S100			48.880	32.620					s
	MOTA	2483	OH2		S100			61.880	19.473	11.767		45.49		
35	ATOM .	2484	OH2		S100			52.770	21.424	26.815		24.43		S
	ATOM	2485	OH2	TIP	S100	5		35.373	29.094	36.197		35.97		s
	MOTA	2486	OH2	TIP	S100	6		40.815	-6.636	4.389	1.00	43.15		S
	ATOM	2487	OH2	TIP	S100	7		44.953	1.286	11.272	1.00	49.45		S
	ATOM	2488	OH2	TIP	\$101	0		21.004	16.168	27.009	1.00	48.51		s
40	ATOM	2489	OH2		S101			47.094	41.786	9.243	1.00	50.10		s
	ATOM	2490	OH2		S101			32.479	2.978	14.158	1.00	49.47		S
		2491		GLC		1		48.557		-12.279		40.72		Ġ Ì
	ATOM					1		48.836		-11.097		38.05		G.
	ATOM	2492		GLC						-11.476		38.09		G
	MOTA	2493		GLC		1 .		49.266						
45	MOTA	2494		GLC		1		49.559		-10.292		33.99		G
	ATOM	2495	C15	GLC	G	1		48.150		-12.257		37.32		G
	ATOM	2496	016	GLC	G	1 .		48.574	15.582	-12.604	1.00	36.74		G
	ATOM	2497	012	GLC	G	2		40.114	-6.634	-6.562	1.00	33.52		G
	ATOM	2498	C11	GLC	G	2			-6.592	-7.404	1.00	31.05		G
50	ATOM	2499		GLC		2		37.712	-6.417	-6.552	1.00	31.56		G
•	ATOM	2500		GLC		2		36.554	-6.406	-7.389		30.70		G
				GLC		2		37.792	-5.109	-5.761		30.03		G
	ATOM	2501								-4.975		29.66		G
	ATOM	2502		GLC		2		36.609	-4.961					
	MOTA	2503		GLC		3		44.030		-13.470		37.90		G
55	MOTA	2504		GLC		3		43.950		-13.690		38.47		G
	MOTA	2505		GLC		3		42.747		-14.579		39.52		G
	ATOM	2506	014	GLC		3		41.551		-13.942		39.39		G
	ATOM	2507.	C15	GLC	G	3		42.878	9.280	-15.934		41.43		G
	ATOM	2508		GLC		3		41.736	9.613	-16.731	1.00	40.78		G
												•		

						•						
	ATOM	2509	012 G	LC G	;	5	40.556	1.005	2.289		45.25	G
	ATOM	2510	C11 G	LC G	;	5	40.966	2.332	1.960		40.56	G
	ATOM	2511	C13 G			5	40.187	3.327	2.814		40.36	G
	ATOM	2512	014 G			5	38.791	3.169	2.572	1.00	40.71	G
5	ATOM	2513	C15 G			5	40.619	4.751	2.464	1.00	40.04	G
3	MOTA	2514	016 G			5	39.885	5.681	3.256	1.00	36.89	G
	ATOM	2515	012 G			6.	36.951	22.702	40.046	1.00	63.04	G
	ATOM	2516	C11 G			6	37.592	21.583	39.422	1.00	62.46	G
		2517	C13 G			6	38.104	21.978	38.030	1.00	61.14	G
10	MOTA	2517	014 G			6	39.034	23.054	38.168	1.00	61.72	, G .
10	ATOM		C15 G			6	36.948	22.429	37.126		60.51	G
	ATOM	2519	O16 G			6	35.992	21.372	36.960		58.61	G
	ATOM	2520	010 G			7	37.316	0.281	14.299		73.45	G
	MOTA	2521				7	37.655	-0.758	15.222		72.78	G
	ATOM	2522	C11 G			7	36.592	-1.856	15.157		72.98	G
15	MOTA	2523	C13 G				35.320	-1.299	15!498		73.88	G
	MOTA	2524	014 6			7	36.924	-2.989	16.134		73.66	G
	MOTA	2525	C15 G			7	36.972	-2.493	17.478		75.38	Ğ
	MOTA	2526	016			7		21.898	5.908		62.51	G
	MOTA	2527	012			8	51.921	20.871	5.063		63.42	G
20	ATOM.	2528	C11 G			8	52.447		3.908		64.28	Ğ
	MOTA	2529	C13 G			8	51.476	20.597 21.794	3.150		66.28	Ğ
	MOTA	2530	014			8	51.297				64.49	Ğ
	MOTA	2531	C15 G			8	50.121	20.137	3.357		64.01	G
	MOTA	2532	016			8	49.233	19.886	29.523		56.89	Ğ
25	MOTA	2533	012			10	36.044	37.499			56.97	G
	ATOM	2534	C11 (10	35.164	36.645	30.259		56.11	G
	ATOM	2535	C13 (10	33.849	36.489	29.494		56.44	G
	ATOM	2536	014	GLC	G	10	33.248	37.772	.29.308		55.84	G
	MOTA	2537	C15 (10	32.900	35.580	30.277		55.39	G
30	MOTA	2538	016	GLC	G	10	31.674	35.442	29.557~		51.49	N
	ATOM	2539	03G Z	ATP	N	1	46.280	25.658	5.170		52.22	N
	MOTA	2540	PG Z	ATP	N	1	46.464	25.053	3.691		51.41	N
	MOTA	2541	01G	ATP	N	1	47.406	23.911	3.763			N
	MOTA	2542	02G		N	1	46.794	26.182	2.784		52.07 51.01	N
35	MOTA	2543	O3B 2	ATP	N	1.	44.976	24.513	3.344		50.20	N
	ATOM	2544	PB :	ATP	N	1	44.560	22.969	3.605			N
	MOTA	2545	O1B	ATP	N	1	43.083	22.898	3.669		49.41	: N
	ATOM	2546	O2B	ATP	N	1	45.345	22.474	4.766		• • •	N
	ATOM	2547	O3A .	ATP	N	1	45.070	22.231	2.255		47.77	N
40	ATOM	2548	PA .	ATP	N	1	45.075	20.613	2.121		42.84	N
	ATOM	2549	O1A	ATP	N	1	45.547	20.291	0.754		43.81	N
	ATOM	2550	O2A	ATP	N	1	45.807	20.035	3.270		45.03	N
	AŤOM	2551	05*	ATP	N	1	43.516	20.223	2.245		37.57	N
	MOTA	2552	C5*	ATP	N	1	42.528	20.925	1.489			N
45	ATOM	2553	C4*	ATP	N	1	41.127	20.379	1.776	1.00	39.45	N.
	ATOM	2554	04*	ATP	N	1	40.907	19.024	1.279		37.72	N N
	ATOM	2555	C3*	ATP	N	1	40.777	20.321	3.251		38.48	N
	ATOM	2556	03*	ATP	N	1	40.360	21.615	3.697		40.42	
	ATOM	2557	C2*	ATP	N	1	39.608	19.374	3.270		37.58	N
50 -		2558	02*	ATP	N	1	38.410	20.076	2.924		35.98	N
	ATOM	2559	C1*	ATP	N	1	39.939	18.346	2.173		35.55	N
	ATOM	2560	N9	ATP	N	1	40.628	17.156	. 2.747		31.76	N
	ATOM	2561		ATP		1	41.864		3.274		30.49	N
	ATOM	2562		ATP		1	42.143	15.877	3.667		29.75	N
55	ATOM	2563		ATP		1	41.088	15.118	3.390		0 27.49	N
"	ATOM	2564	C4	ATP		1	40.125	15.925	2.810		0 30.02	N
	ATOM	2565		ATP		1	38.937	15.389			0 27.11	N
	ATOM	2566		ATP		1	38.679	14.085			0 25.62	N
	ATOM	2567		ATP		1	39.597	13.283	3.175	1.0	0 21.76	N

									12 769	3.571	1 00	23.90	N
	MOTA	2568	C6	ATP 1		. 1	•	40.800	13.768	4.127		21.94	N
	ATOM	2569	Иб	ATP I		1		41.698	12.964	-0.639		56.05	I
	MOTA	2570	S	SO4		1		58.680	8.493	0.483		58.83	I
	MOTA	2571	01	SO4		1		57.956	7.875	-1.188		57.04	Ī
5	MOTA	2572	02	SO4		1		57.886	9.607	-1.683		57.47	ī
	ATOM	2573	03	SO4		1		58.906	7.478	-0.156		57.51	I
	ATOM	2574	04	SO4		1		59.976	9.008	7.057		84.24	Ĩ
	ATOM	2575	S		Ι	2		39.339	4.855	7.711		85.02	Ī
	ATOM	2576	01		I	2		39.390	6.175	5.797		84.75	Ī
10	MOTA	2577	02		I	2		40.101	4.897	6.766		84.94	I
	MOTA	2578	03		Ţ	2		37.936	4.506	7.954		84.44	Ī
	MOTA	2579	04		I	2		39.931	3.842	3.310	1.00	58.58	ī
-	ATOM	2580	S	SO4		3		38.987	-2.256	3.827		59.11	I
	ATOM	2581	01		I	3		37.734	-1.675	2.172		59.91	I
15	ATOM	2582	02		I	3		39.460	-1.454	2.866		60.97	I
	MOTA	2583	03	SO4		3		38.743	-3.640	4.369		59.58	I
	MOTA	2584	04	SO4		3		40.014	-2.260 5.289	30.981	1.00	64.34	I
	MOTA	2585	S		I	4		34.397	6.528	30.742	1.00	60.43	I
	MOTA	2586	01		I	4		33.627	4.427	29.782	1.00		I
20	MOTA	2587	02	SO4	I	4		34.337	4.572	32.133	1.00		I
	ATOM	2588	03	SO4	I	4		33.816	5.626	31.277		63.55	I
	ATOM	2589	04	SO4	I	4		35.806 55.074	-6.984	-3.711	1.00		I
	ATOM	2590	S	SO4	I	5		54.657	-7.518	-2.399	1.00		I
	MOTA	2591	01	SO4	I	5		54.209	-5.845	-4.065	1.00		I
25	MOTA	2592	02		I	5		54.209	-8.034	-4.742	1.00		I
	MOTA	2593	03		I	5 5		56.477	-6.532	-3.633	1.00	75.15	I
	MOTA	2594	04	SO4	I	_		57.362	24.998	13.149	1.00	66.76	P
	MOTA	2595	02			100 100		59.399	26.166	13.761	1.00		P
	MOTA	2596	03	PO4		100		57.761	25.606	15.462	1.00	67.43	P
30	MOTA	2597	04	PO4		100		57.264	27.325	13.818	1.00	65.91	P
	MOTA	2598	01	PO4 PO4		100		57.947	26.025	14.048	1.00	66.69	P
	ATOM	2599	P	204	r	100		3 3					
	END											•	

Example 4: Co-ordinates for the dimer of the PDK1 fragment, without alternate side chains. Chain A is the molecule for which co-ordinates are given in Examples 2 and 3, and chain B is the symmetry-related molecule.

40 45 50	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1 2 3 4 5 6 7 8 9 10 11 12 13 14	CB CG CO NCD CA NCD CCA CB CG CO NCD	PRO A	72 72 72 73	58.912 59.621 59.493 59.196 60.984 60.554 60.040 59.356 59.712 58.840 58.672 59.796 57.527 56.710 57.341	-7.251 -6.941 -6.506 -5.318 -6.073 -5.762 -7.035 -7.385 -8.816 -6.986 -8.321 -9.133 -6.208 -6.451 -5.268 -4.454	8.216 9.534 5.894 5.766 7.833 9.207 7.217 4.890 4.898 3.578 2.858 3.419 3.673 4.561 2.753 2.708	1.00 67.78 1.00 69.16 1.00 67.06 1.00 66.66 1.00 67.86 1.00 67.75 1.00 66.32 1.00 67.17 1.00 65.61 1.00 66.47 1.00 67.57 1.00 63.94 1.00 64.11 1.00 61.57 1.00 58.74	A A A A A A A A A A A A A A A A A A
55	ATOM ATOM	16 17	CA CB	ALA A ALA A	73 73	56.133 56.438	-4.454 -3.030	3.165	1.00 58.05	A

		•									
	ATOM	18	С	ALA A	73		55.626	-4.448	1.271	1.00 56.78	A
	ATOM	19	0	ALA Á	73		56.347	-4.834	0.349	1.00 56.95	A
	ATOM	20	N	PRO A	74		54.372	-4.024	1.057	1.00 54.15	A
	ATOM	21	CD	PRO A	74		53.335	-3.610	2.018	1.00 53.31	A
5	ATOM	22	CA	PRO A	74		53.856	-4.003	-0.314	1.00 52.54	. A
•	ATOM	23	CB	PRO A	74		52.474	-3.375	-0.148	1.00 52.86	A
	ATOM	24	CG	PRO A	74		52.067	-3.824	1.226	1.00 52.88	A
	ATOM	25	С	PRO A	74		54.772	-3.167	-1.204	1.00 50.08	A
	ATOM	26	0	PRO A	74		55.559	-2.361	-0.708	1.00 49.96	·A
10	ATOM	27	N	ALA A	75		54.680	-3.366	-2.514	1.00 47.58	A
	ATOM	28	CA	ALA A	75		55.503	-2.602	-3.446	1.00 44.69	A
	ATOM	29	СВ	ALA A	75		55.312	-3.121	-4.870	1.00 46.14	A
	ATOM	30	С	ALA A	75		55.100	-1.134	-3.371	1.00 41.55	A
	ATOM	31	0	ALA A	75		53.947	-0.813	-3.086	1.00 41.01	A
15	ATOM	32	N	LYS A	76		56.053	-0.245	-3.619	1.00 38.31	A
13	ATOM	33	CA	LYS A	76		55.781	1.184	-3.588	1.00 35.72	A
	ATOM	34	СВ	LYS A	76		57.053	1.957	-3.930	1.00 37.70	A
	ATOM	35	CG	LYS A	76		57.123	3.356	-3.350	1.00 40.99	A
	ATOM	36	CD	LYS A	76		57.262	3.316	-1.836	1.00 40.04	A
20	ATOM	37	CE	LYS A	76		57.511	4.705	-1.277	1.00 42.08	A
20	ATOM	38	ΝZ	LYS A	76		57.681	4.695	0.202	1.00 42.99	A
	ATOM	39	C	LYS A	76		54.708	1.467	-4.638	1.00 32.65	A
	ATOM	40	ō	LYS A	76		54.814	1.005	-5.770	1.00 31.41	A
	ATOM	41	N	LYS A	77		53.668	2.207	-4.270	1.00 28.59	A
25	ATOM	42	CA	LYS A	77		52.619	2.517	-5.232	1.00 25.72	A
2.5	ATOM	43	CB	LYS A	77		51.316	2.865	-4.509	1.00 26.22	A
	ATOM	44	CG	LYS A	77		50.796	1.731	-3.631	1.00 27.15	A
	ATOM	45	CD	LYS A	77		49.487	2.089	-2.967	1.00 26.80	A
	ATOM	46	CE	LYS A	_		49.136	1.091	-1.870	1.00 27.31	A
30	ATOM	47	ΝZ	LYS A			48.998	-0.296	-2.380	1.00 27.17	A
30	ATOM	48	C	LYS A			53.053	3.668	-6.137	1.00 24.67	A
	ATOM	49	Ö	LYS A			54.010	4.377	-5.829	1.00 21.60	. A
	ATOM	50	Ŋ	ARG A			52.351	3.838	-7.254	1.00 23.66	A
	ATOM	51	CA	ARG A			52.662	4.897	-8.211	1.00 26.14	A
35	ATOM	52	CB	ARG A			53.574	4.344	-9.318	1.00 28.57	A
22	ATOM	53	CG	ARG A			53.017	3.139	-10.050	1.00 34.78	A
	ATOM	54	CD	ARG A		· .	54.092		-10.896	1.00 40.96	A
	ATOM	55	NE	ARG A			53.560	1.364	-11.700	1.00 48.93	A
	ATOM	56	CZ	ARG A			52.985	0.270	-11.203	1.00 52.58	A
40	ATOM	57		L ARG A			52.860	0.113	-9.889	1.00 54.60	A
40	ATOM	58		ARG A			52.530	-0.672	-12.022	1.00 54.09	A
	ATOM	59	C	ARG A			51.382	5.488	-8.803	1.00 23.76	A
	ATOM	60	ő	ARG A			50.311	4.888	-8.706	1.00 24.25	Α,
	ATOM	61	N	PRO A			51.475	6.676	-9.428	1.00 21.76	A
45	ATOM	. 62	ÇD	PRO A			52.691	7.475	-9.668	1.00 20.82	A
73	ATOM	63	CA	PRO A			50.301	7.325	-10.021	1.00 21.96	A
	ATOM	. 64	CB	PRO A			50.910	8.481	-10.816	1.00 22.27	A
	ATOM	65	CG	PRO A			52.124	8.831	-10.014	1.00 22.12	A
	ATOM	66	C	PRO A			49.446	6.413	-10.903	1.00 22.86	A
50	ATOM	67	ő	PRO A			48.213	6.461	-10.842	1.00 20.52	A
, 50	ATOM	68	N	GLU A			50.103		-11.714	1.00 21.87	A
	ATOM	69	CA	GLU P			49.403	4.685	-12.628	1.00 22.99	A
	ATOM	70	CB	GLU F			50.393	3.994	-13.571	1.00 25.24	A
		70	CG	GLU F			51.230	2.907	-12.925	1.00 28.75	A
55	ATOM	72	CD				52.157	2.224	-13.913	1.00 31.99	A
33	ATOM	73		1 GLU F			53.072	2.897	-14.433	1.00 34.34	A
	ATOM	74		2 GLU F			51.969	1.015	-14.172	1.00 32.83	A
	ATOM			GLU F			48.556	3.631	-11.912	1.00 22.09	A
	ATOM	75 76		GLU A			47.692		-12.530	1.00 22.37	A
	ATOM	70	U	ء صدق							

	, ATOM	77	N	ASP A	81	48.804	3.413 -10.622	1.00 19.97	A
	MOTA	78	CA	ASP A	81	48.026	2.423 -9.874	1.00 19.93	A
	ATOM	79	CB	ASP A	81	48.736	2.029 -8.571	1.00 21.19	A
	ATOM	80	CG	ASP A	81	50.089	1.380 -8.807	1.00 22.46	A
5	ATOM	81	OD1	ASP A	81	50.195	0.554 -9.731	1.00 24.22	Α
-	· ATOM	82		ASP A	81	51.043	1.685 -8.058	1.00 23.33	A
	ATOM	83	С	ASP A	81	46.652	2.975 -9.518	1.00 20.85	A
	ATOM	84	0	ASP A	81	45.793	2.246 -9.015	1.00 19.96	A
	ATOM	85	N	PHE A	82	46.445	4.258 -9.804	1.00 18.91	A
10	ATOM	86	CA	PHE A	82	45.200	4.934 -9.465	1.00 19.30	A
10	ATOM	87	СВ	PHE A	82	45.475	6.027 -8.427	1.00 18.43	A
•	ATOM	88		PHE A	82	46.134	.5.531 -7.175	1.00 18.01	A
	ATOM	89		PHE A		45.371	5.136 -6.084	1.00 17.19	A
	ATOM	90		PHE A		47.520	5.460 -7.086	1.00 18.99	A
15	ATOM	91		PHE A		45.977	4.676 -4.918	1.00 17.12	A
13	ATOM	92		PHE A		48.137	5.000 -5.925	1.00 19.64	· А
	ATOM	93	CZ	PHE A		47.361	4.607 -4.838	1.00 18.00	A
	ATOM	94	C	PHE A		44,476	5.596 -10.621	1.00 20.81	Α
	ATOM	95	Ö	PHE A		45.066	5.933 -11.649		Α
20	ATOM	96	N	LYS A		43.182	5.792 -10.411	1.00 19.80	Α
20		90 97	CA	LYS A		42.321	6.478 -11.353		A
	ATOM ATOM	98	CB	LYS A		41.096	5.625 -11.687	1.00 22.02	À
		99	CG	LYS A		40.062	6.326 -12.550		. A
	ATOM	100	CD	LYS A		38.974	5.355 -12.981		Α
25	ATOM		CE	LYS. A		37.909	6.042 -13.824		A
25	ATOM	101 102	NZ	LYS A		37.179	7.086 -13.043		A
	ATOM		. C	LYS A		41.913	7.702 -10.541		A
	MOTA	103		LYS A		41.084	7.606 -9.635		A
	. ATOM	104	0	PHE A		42.513	8.848 -10.835		A
20	MOTA	105 106	N CA	PHE A		42.188	10.049 -10.083		A
30	MOTA	107	CB	PHE A		43.279	11.103 -10.258		A
	MOTA	107	CG	PHE A		44.571	10.741 -9.587		A
	MOTA	100		PHE A		45.498	9.926 -10.224		A
	ATOM ATOM	110		PHE A			11.183 -8.299		A
35	ATOM	111		PHE A		46.676	9.556 -9.589	1.00 18.09	Α
33	ATOM	112		PHE A		46.021	10.816 -7.653	1.00 18.89	A
	ATOM	113	CZ	PHE A		46.936	10.002 -8.301	1.00 17.33	A
	ATOM	114	C	PHE A		40.834	10.617 -10.460	1.00 19.69	A
	ATOM	115	Ö	PHE A		40.391	10.489 -11.601		Α
40	ATOM	116	N	GLY A		40.178	11.233 -9.484		A
40	ATOM	117	CA	GLY A		38.872	11.810 -9.716		A
	ATOM	118	C	GLY A		38.819	13.280 -9.346	1.00 18.75	, A
	ATOM	119	Ö	GLY A		39.740	14.043 -9.650	1.00 18.45	A
	ATOM	120	N	LYS A		37.753	13.673 -8.659	1.00 16.00	A
45	ATOM	121	CA	LYS A		37.571	15.064 -8.278		A
43	ATOM	122	СВ	LYS A		36.133	15.302 -7.812		Α
	ATOM	123	CG	LYS A		35.793	14.660 -6.481	. 1.00 21.55	Α
	ATOM	124	CD	LYS A		34.368	14.981 -6.066	1.00 26.48	A
	ATOM	125	CE	LYS A		33.994	14.239 -4.793	3 1.00 31.92	Α
50	ATOM	126	NZ	LYS F		32.568	14.457 -4.412	1.00 35.36	A
50	ATOM	127	C	LYS F		38.523	15.571 -7.202	1.00 18.57	A
	ATOM	128	Ö	LYS F		39.045	14.807 -6.385	•	A
	ATOM	129	N	ILE A		38.737	16.881 -7.227	1.00 17.88	Α
	ATOM	130	CA	ILE P		39.577	17.554 -6.256	1.00 18.26	A
55	ATOM	131	CB	ILE F		39.994	18.952 -6.772	1.00 19.60	A
,,	ATOM	132		ILE F		40.593	19.786 -5.628	1.00 18.73	A
	ATOM	133		ILE A			18.786 -7.945	1.00 21.16	A
	ATOM	134		ILE A			20.087 -8.588	1.00 25.26	Α
	ATOM	135	C	ILE A			17.709 -4.99		A
	AION	100	•		- 0.				

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	ATOM	136	0	ILE	A	87		37.628	18.249	-5.052	1.00 20.41	Α
	ATOM	137	N	LEU	Α	88		39.240	17.229	-3.867	1.00 19.15	A
	ATOM '	138	CA	LEU	Α	88		38.508	17.324	-2.611	1.00 20.68	A
	MOTA	139	СВ	LEU	Α	88		38.870	16.151	-1.700	1.00 19.97	А
5	ATOM	140	CG	LEU	Α	88		38.529	14.759	-2.237	1.00 19.24	, A
	ATOM	141	CD1			88		39.090	13.692	-1.311	1.00 21.41	A
	ATOM	142	CD2	LEU	Α	88		37.029	14.622	-2.359	1.00 18.84	A
	MOTA	143	С	LEU	Α	88		38.815	18.632	-1.901	1.00 23.11	A
	ATOM	144	0	LEU	Α	88		37.999	19.146	-1.139	1.00 25.10	A
10	ATOM	145	N	GLY	Α	89		39.997	19.174	-2.149	1.00 24.09	A
	ATOM	146	CA	GLY	Α	89		40.367	20.418	-1.507	1.00 24.27	Α
	ATOM	147	С	GLY	A	89		41.658	20.954	-2.078	1.00 25.47	A
	MOTA	148	0	GLY	Α	89		42.445	20.202	-2.666	1.00 22.19	A
	ATOM	149	N	GLU	Α	90		41.870	22.254	-1.906	1.00 26.22	A
15	MOTA	150	CA	GLU	Α	90		43.064	22.924	-2.404	1.00 29.96	A
	MOTA	151	СВ	GLU	Α	90		42.698	23.814	-3.596	1.00 30.75	A
	MOTA	152	CG	GLU	Α	90		42.267	23.038	-4.831	1.00 34.32	A
	MOTA	153	CD	GLU	Α	90		41.711	23.930	-5.927	1.00 38.27	A
	MOTA	154	OE1	GLU	Α	90		40.590	24.456	-5.764	1.00 40.57	A
20	ATOM	155	OE2	GLU	Α	90		42.398	24.110	-6.952	1.00 40.90	A
	MOTA	156	С	GLU	Α	90		43.711	23.768	-1.313	1.00 30.68	A
	MOTA	157	0	GLU	Α	90		43:049	24.574	-0.668	1.00 32.83	A
	ATOM	158	N	GLY	Α	91		45.006	23.566	-1.104	1.00 29.66	A
	ATOM	159	CA	GLY	Α	91		45.724	24.332	-0.104	1.00 29.40	A
25	ATOM	160	С	GLY	Α	91		46.795	25.151	-0.798	1.00 29.98	A
	ATOM	161	0	GLY		91		46.894	25.130	-2.028	1.00 28.16	A
	ATOM .	162	N	SER	Α	92		47.605	25.870	÷0.029	1.00 28.30	A
	ATOM	163	CA	SER	Α	92		48.653	26.681	-0.633	1.00 30.50	A
	ATOM	164	CB	SER	A	92		49.165	27.717	0.370	1.00 32.43	А
30	ATOM	165	OG	SER	Α	92		49.520	27.099	1.593	1.00 40.94	A
	ATOM	166	С	SER	Α	92		49.815	25.843	-1.164	1.00 29.77	A
	ATOM	167	0	SER	A	92		50.456	26.221	-2.143	1.00 30.46	А
	ATOM	168	N	PHE	Α	93		50.087	24.703	-0.536	1.00 27.65	A
	ATOM	169	CA	PHE	Α	93		51.185	23.855	-0.995	1.00 26.34	A
35	ATOM	170	CB	PHE	Α	93		52.281	23.785	0.068	1.00 27.95	A
	ATOM	171	CG	PHE	Α	93		52.861	25.117	0.406	1.00 31.06	A
	ATOM	172	CD1	PHE	Α	93		52.283	25.909	1.392	1.00 29.96	A
	ATOM	173	CD2	PHE	A	93		53.949	25.613	-0.308	1.00 31.38	A
	ATOM	174	CE1	PHE	A	93		52.779	27.181	1.665	1.00 32.69	A
40	ATOM	175	CE2	PHE	Α	93		54.452	26.883	-0.044	1.00 32.63	A
	ATOM	176	CZ	PHE	A	93		53.864	27.670	0.945	1.00 31.81	A
	ATOM	177	С	PHE	A	93		50.759	22.445	-1.365	1.00 25.39	A
	ATOM	178	0	PHE	A	93		51.601	21.559	-1.522	1.00 24.59	A
	ATOM	179	N	SER	Α	94		49.457	22.235	-1.519	1.00 23.63	A
45	ATOM	180	CA	SER	Α	94		48.965	20.912	-1.860	1.00 21.43	A
	ATOM	181	CB	SER		94		49.017	20.013	-0.628	1.00 21.42	A
	ATOM	182	OG	SER		94		48.091	20.475	0.340.	1.00 21.19	A
	ATOM	183	С	SER		94		47.539	20.925	-2.378	1.00 19.82	Α
	ATOM	184	0	SER		94		46.795	21.882	-2.173	1.00 18.76	A
50	ATOM	185	N	THR		95	•	47.174	19.832	-3.038	1.00 19.38	A
	ATOM	186	CA	THR		95		45.840	19.637	-3.580	1.00 17.98	A
	ATOM	187	CB	THR		95		45.818	19.818	-5.110	1.00 19.25	A
	ATOM	188	OG1	THR		95		46.196	21.162	-5.434	1.00 22.04	A
	ATOM	189		THR		95		44.421	19.549	-5.661	1.00 17.61	A
55	ATOM	190	С	THR		95		45.455	18.201	-3.243	1.00 18.61	A
	ATOM	191	O.	THR		95.		46.212	17.264	-3.524	1.00 17.10	A
	ATOM	192	Ŋ	VAL		96		44.295	18.024	-2.623	1.00 16.53	A
	ATOM	193	CA	VAL		96		43.845	16.685	-2.266	1.00 16.05	A
	ATOM	194	СВ	VAL		96		43.170	16.672	-0.886	1.00 16.32	A

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	ATOM	195	CG1	VAL	A	96		42.7.41	15.249	-0.532	1.00 18.02	Α
	MOTA	196	CG2	VAL	Α	96		44.145	17.206	0.168	1.00 16.69	A
	MOTA	197	С	VAL	А	96		42.875	16.207	-3.335	1.00 16.42	A
	MOTA	198	0	VAL	Α	96		41.906	16.892	-3.665	1.00 16.47	A
5	ATOM	199	N	VAL		97		43.157	15.033	-3.888	1.00 16.80	A
	ATOM	200	CA	JAV		97		42.338	14.471	-4.949	1.00 16.72	A
	ATOM	201	CB	VAL	A	97		43.153	14.354	-6.255	1.00 18.43	A
	MOTA	202		VAL		97		42.249	13.927	-7.404	1.00 19.69	A
	ATOM	203		VAL		97		43.831	15.685	-6.569	1.00 17.84	A
10	ATOM	204	С	VAL	A	97		41.812	13.091	-4.583	1.00 16.77	A
	ATOM	205	0	VAL		97		42.532	12.270	-4.014	1.00 17.13	A
	ATOM	206	N	LEU	A	98		40.545	12.845	-4.895	1.00 16.62	A
	ATOM	207	CA	LEU	A	98		39.947	11.548	-4.624	1.00 17.04	A
	ATOM	208	CB	LEU		98		38.424	11.633	-4.743	1.00 16.89	A
15	ATOM	209	CG	LEU		98		37.635	10.342	-4.508	1.00 19.46	Α
	MOTA	210		LEU		98		37.990	9.762	-3.146	1.00 20.07	A
	MOTA	211		PEA		98		36.143	10.627	-4.588	1.00 17.93	A
	MOTA	212	С	LEU		98		40.512	10.597	-5.677	1.00 17.38	A
	MOTA	213	0	LEU		98	_	40.527	10.920	-6.863	1.00 18.60	A
20	MOTA	214	N	ALA		99		40.995	9:438	-5.246	1.00 17.13	A
	MOTA	215	CA	ALA		99		41.570	8.466	-6:168	1.00 18.42	A ·
	ATOM	216	CB	ALA		99		43.090	8.524	-6.105	1.00 14.76	A
	MOTA	217	С	ALA		99		41.102	7.055	-5.848	1.00 21.40	A
	MOTA	218	0	ALA		99		40.941	6.691	-4.679	1.00 22.52	A
25	ATOM	219	N	ARG	-			40.878	6.261	-6.888	1.00 19.77 1.00 20.85	A A
	ATOM	220	CA	ARG				40.459	4.884	-6.693		A
	ATOM	221	CB	ARG				39.202	4.585 3.205	-7.518 -7.256	1.00 24.22 1.00 31.78	A
	MOTA	222	CG .	ARG				38.608 37.326	2.979	-8.048	1.00 31.78	A
20	ATOM	223	CD	ARG				36.213	3.818	-7.594	1.00 30.24	A
30	ATOM	224	NE	ARG ARG				35.566	3.662	-6.439	1.00 42.05	A
	MOTA	225	CZ	ARG				35.912	2.696	-5.598	1.00 40.67	A
	MOTA	226 227		ARG				34.559	4.468	-6.128	1.00 43.65	A
	ATOM ATOM	228	C	ARG				41.613	3.985	-7.129	1.00 18.63	A
35 -	ATOM	229	o	ARG				42.078	4.065	-8.271	1.00 19.49	A
35 .	MOTA	230	N			101		42.102	3.157	-6.212	1.00 16.43	A
	ATOM	231	CA			101		43.196	2.246	-6.533	1.00 16.11	A
	ATOM	232	CB			101		43.774	1.637	-5.248	1.00 16.79	Α
	ATOM	233	CG	GLU				44.917	0.657	-5.488	1.00 16.51	A
40	ATOM	234	CD			101		45.501	0.115	-4.200	1.00 18.20	A
	ATOM	235		GLU				44.733	-0.081	-3.239	1.00 18.32	A
	ATOM	236	OE2	GLU	Α	101		46.725	-0.132	-4.150	1.00 17.14	A
	ATOM	237	С	GLU	Α	101		42.625	1.152	-7.442	1.00 17.92	Α
	ATOM	238	0	GLU	Α	101		41.681	0.462	-7.069	1.00 18.02	A
45	ATOM	239	N	LEU	A	102		43.198	1.002	-8.632	1.00 19.06	A
	ATOM	240	CA	LEU	.A	102		42.718	0.025	-9.607	1.00 20.71	A
	ATOM	241	CB	LEU	Α	102		43.569		-10.878	1.00 23.42	. A
	ATOM	242	CG	LEU	Α	102		43.531	1.426	-11.642	1.00 25.30	Α
	ATOM	- 243	CD1	LEU	A	102		44.57.7		-12.748	1.00 27.88	A
50	ATOM	244	CD2	LEU				42.140		-12.214	1.00 26.79	. A
	ATOM	245	С			102	-	42.671	-1.418	-9.125	1.00 21.62	· A
	ATOM	246	0			102		41.668	-2.103	-9.305	1.00 21.09	A
	ATOM	247	N			103		43.753	-1.874	-8.507	1.00 19.38	A
	ATOM	248	CA	ALA				43.836	-3.249	-8.035	1.00 20.87	A
55	ATOM	249	CB	ALA				45.284	-3.571	-7.671	1.00 19.23	A
	MOTA	250	С			103		42.919	-3.629	-6.872	1.00 19.92	
	ATOM	251	0			103		42.703	-4.815	-6.628	1.00 20.38	A
	ATOM	252	N			104		42.361	-2.643	-6.175	1.00 18.12	
	ATOM	,253	CA	THR	A	104		41.517	-2.927	-5.018	1.00 17.15	A

	ATOM	254	СВ	THR	Α	104	42,212	-2.484	-3.717	1.00	19.54	A
•	ATOM	255		THR			42.456	-1.070	-3.773		19.26	A
	ATOM	256		THR			43.536	-3.219	-3.529		17.02	A
	ATOM	257	C	THR			40.159	-2.247	-5.026		19.44	A
5	ATOM	258	Ö	THR			39.259	-2.648	-4.285		18.70	Ā
,	ATOM	259	N	SER			40.034	-1.207	-5.847		19.65	A
				SER			38.819	-0.400	-5.967		19.37	A
	ATOM	260	CA					-1.304	-6.173		21.81	A
	ATOM	261	CB	SER			37.598					
	ATOM	262	OG	SER			36.431	-0.539	-6.412		23.01	A A
10	MOTA	263	C	SER			38.644	0.447	-4.701		18.99	
	MOTA	264	0	SER			37.602	1.070	-4.488		18.66	A
	MOTA	265	N	ARG			39.674	0.468	-3.861		16.84	A
	MOTA	266	CA	ARG			39.655	1.267	-2.634		16.21	A
	MOTA	267	CB	ARG			40.827	0.886	-1.723		16.41	A
15	ATOM	268	CG	ARG			40.619	-0.367	-0.906		15.49	A
	MOTA	269	CD	ARG			41.887	-0.755	-0.170		17.43	Α
	MOTA	270	NE	ARG			41.620	-1.792	0.824		20.47	A
	MOTA	271	CZ	ARG			42.548	-2.568	1.371		20.24	A
	MOTA	272	NH1	ARG	Α	106	43.821	-2.433	1.017		17.80	A
20	ATOM	273	NH2	ARG	Α	106	42.198	-3.468	2.285		20.14	A
	ATOM	274	С	ARG	Α	106	39.785	2.746	-2.981		17.37	A
	MOTA	275	0	ARG	A	106	40.514	3.103	-3.902	1.00	17.75	A
	ATOM	276	N	GLU	Α	107	39.085	3.599	-2.240		16.06	A
	ATOM	277	CA	GLU	Α	107	39.156	5.039	-2.461		20.80	A
25	ATOM	278	СВ	GLU	Α	107	37.779	5.694	-2.337	1.00	22.93	A
	ATOM	279	CG	GLU	Α	107	36.711	5.171	-3.269	1.00	30.87	Α
	ATOM	280	CD	GLU	Α	107	35.431	5.975	-3.148	1.00	32.40	Α
	ATOM	281	OE1	GLU	A	107	35.262	6.939	-3.923	1.00	33.74	A
	ATOM	282	OE2	GLU	Α	107	34.608	5.654	-2.263	1.00	36.00	Α
30	ATOM	283	С	GLU			40.053	5.678	-1.410	1.00	18.93	Α
	ATOM	284	0	GLU	Α	107	39.891	5.427	-0.220	1.00	19.21	A
	ATOM	285	N	TYR	Α	108	40.988	6.507	-1.852	1.00	16.70	Α
	ATOM	286	CA	TYR	A	108	41.883	7.209	-0.942	1.00	15.86	Α
	ATOM	287	СВ	TYR			43.325	6.728	-1.104	1.00	15.30	A
35	ATOM	288	CG	TYR	Α	108	43.593	5.328	-0.612	1.00	16.33	Α
-	ATOM	289	CD1				43.765	5.066	0.746	1.00	16.36	A
	MOTA	290		TYR			44.046	3.769	1.201	1.00	18.48	Α
	ATOM	291	CD2	TYR			43.701	4.268	-1.511	1.00	13.25	Α
	ATOM	292	CE2	TYR			43.980	2.981	-1.075	1.00	17.28	Α
40	ATOM	293	CZ	TYR			44.152	2.736	0.276	1.00	19.17	Α
,,	ATOM	294	ОН	TYR	Α	108	44.440	1.461	0.688	1.00	19.38	A
	ATOM	295	C	TYR	A	108	41.850	8.687	-1.292	1.00	16.80	A
	ATOM	296	ō	TYR			41.560	9.058	-2.431	1.00	15.22	A
	ATOM	297	N	ALA			42.132	9.528	-0.306	1.00	14.61	A
45	MOTA	298	CA				42.207		-0.539	1.00	14.30	Α
	ATOM '	299	CB	ALA			41.671	11.726	0.661	1.00	14.78	A
	ATOM	300	C	ALA			43.713	11.136	-0.667	1.00	16.79	A
	ATOM	301	ō	ALA			44.450	10.983	0.317		16.52	Α
	ATOM	302	N	ILE			44.182	11.410	-1.881		14.80	Α
50	ATOM	303	CA	ILE			45.609		, -2.093	1.00	15.80	A
50	ATOM	304	CB	ILE			46.065	10.863	-3.396		16.85	A
	ATOM	305	CG2				47.550	11.098	-3.632	1.00	16.80	A
	ATOM	306		ILE			45.774	9.358	-3.284		17.76	A
	ATOM	307		ILE			46.308	8.513	-4.437		16.07	A
55	ATOM	307	CDI	ILE			46.004	13.045	-2.129		17.78	· A
55	ATOM	309	Ö	ILE			45.534	13.813	-2.976		16.24	A
		310	Ŋ	LYS			46:846	13.435	-1.177		16.15	A
	ATOM	311	CA	LYS			47.326	14.808	-1.100		17.20	A
	ATOM	312	CB	LYS			47.700	15.176	0.344		17.41	A
	ATOM	214	CD	טוע	47		47.700	10.110	0.011			

							•	77.		·	••
	ATOM	313	CG	LYS	A 11:	48.350	16.547	0.464	1.00	20.71	. A
	ATOM	314	CD	LYS	A 11:	48.585	16.971	1.910	1,00	24.25	A
	ATOM	315	CE		A 11:	47.288	17.381	2.598		29.46	A
	ATOM	316	NZ		A 11:	47.516	17.866	4.000		30.50	A
5	ATOM	317	С	LYS		48.551	14.890	-1.994		16.41	A
,	ATOM	318	Õ	LYS		49.509	14.137	-1.813		18.20	
		319			A 112						A
	ATOM		N	•		48.509	15.798	-2.963		15.87	A
	ATOM	320	CA		A 112	49.606	15.967	-3.907		17.28	A
	ATOM	321	CB		A 112	49.079	15.911	-5.358		16.43	A
10	ATOM	322		ILE		50.235	15.998	-6.341		15.12	A
	ATOM	323	CG1	ILE .		48.293	14.609	~5.565		16.82	A
	ATOM	324		ILE .		47.500	14.511	-6.904		18.47	A
	ATOM	325	С	ILE .		50.307	17.301	-3.663	1.00	19.03	A
	ATOM	326	0	ILE .	A 112	49.669	18.350	-3.635	1.00	19.15	· A
15	ATOM	327	N	LEU .	A 113	51.622	17.245	-3.472	1.00	20.22	Α
	ATOM	328	CA	LEU .	A 113	52.416	18.442	-3.214	1.00	22.36	A
	ATOM	329	CB	LEU .	A 113	52.995	18.397	-1.794	1.00	22.13	Α
	ATOM	330	CG	LEU .	A 113	52.042	18.063	-0.646	1.00	22.46	A
	ATOM	331	CD1	LEU .	A 113	51.866	16.557	-0.553	1.00	23.81	A
20	ATOM	332		LEU		52.603	18.595	0.660		23.68	A
20	ATOM	333	C	LEU		53.560	18.547	-4.215		23.37	A
	ATOM	334	ō	LEU		54.300	17.586	-4.424		23.11	A
	ATOM	335	N	GLU .		53.706	19.714	-4.834		23.88	A
	•	336	CA	GLU .		54.771	19.920	-5.806		26.00	A
25	ATOM	337	CB	GLU .		54.435	21.111	-6.706		27.74	Ā
25	ATOM									35.07	A ·
	ATOM	338	CG	GLU .		55.533	21.452	-7.696		39.24	
	ATOM	339	CD	GLU .		55.220	22.696	-8.497			A
	ATOM	340		GLU .		54.808	23.703	-7.885		41.45	A
	ATOM	341		GLU .		55.395	22.670	-9.736		44.05	A
30	ATOM	342	С	GLU .		56.087	20.163	-5.067		24.37	A
	ATOM	343	0	GLU .		56.186	21.071	-4.238		24.43	, A
	ATOM	344	N	LYS .		57.096	19.350	-5.360		24.10	A
	ATOM	345	CA	LYS .	A 115	58.376	19.493	-4.678		24.93	Α
	MOTA	346	CB	LYS .		59.339	18.373	-5.103		23.72	A
35	ATOM	347	,CG	LYS ,	A 115	59.139	17.080	-4.308		23.09	A
	ATOM	348	CD	LYS .	A 115	60.064	15.944	-4.743		21.92	A
	ATOM	349	CE	LYS .	A 115	59.691	15.400	-6.117	1.00	22.42	A
	ATOM	350	NZ	LYS .	A 115	60.447	14.150	-6.448		19.71	A
	ATOM	351	С	LYS :	A 115	59.031	20.858	-4.868	1.00	26.87	A
40	ATOM	352	0	LYS .	A 115	59.492	21.469	-3.903	1.00	26.17	A
	ATOM	353	N	ARG .	A 116	59.058	21.348	-6.102	1.00	28.73	A
	ATOM	354	CA	ARG :	A 116	59.678	22.638	-6.380	1.00	29.66	A
	ATOM	355	СВ	ARG .	A 116	59.533	22.980	-7.868	1.00	31.29	A
	ATOM	356	CG	ARG	A 116	60.047	24.361	-8.267	1.00	33.19	A
45	ATOM	357	CD	ARG	A 116	61.368	24.710	-7.590	1.00	35.13	· A
	ATOM	358	NE	ARG		62.329	23.612	-7.618		36.42	Α
	ATOM	359	CZ	ARG .		63.510	23.648	-7.009		36.18	A
	ATOM	360		ARG		63.871	24.729	-6.332		36.12	A
	ATOM	361		ARG		64.324	22.602	-7.067		35.77	A
50	ATOM	362	C	ARG A		59.097	23.761	-5.519		29.70	A
50		363				59.843	24.515	-4.889		29.16	A
	ATOM		0	ARG		57.773	23.862	-5.472		27.22	A
	ATOM	364	N	HIS						26.33	
	ATOM	365	CA	HIS		57.126	24.903 24.835	, -4.681		28.41	A A
	ATOM	366	CB	HIS		55.606		-4.848			A A
55	ATOM	367	CG	HIS		54.881	26.005	-4.258		31.82	A
	MOTA	368		HIS I		55.309	27.249	-3.935		33.19	A
	ATOM	369		HIS		53.536	25.974	-3.961		34.30	A
	MOTA	370		HIS I		53.165	27.148	-3.480		34.58	· A
	ATOM	371	NE2	HIS	A 117	54.222	27.940	-3.455	1.00	35.18	A

	ATOM	372	С	HIS .	A 117		57.47.7	24.780	-3.202	1.00	26.22	A
	ATOM	373	0	HIS .	A 117		57.737	25.776	-2.534		25.67	· A
	ATOM	374	N	ILE .	A 118		57.469	23.554	-2.689	1.00	24.94	A
	ATOM	375	CA	ILE :	A 118		57.792	23.315	-1.285	1.00	23.94	A
5	ATOM	376	CB	ILE 2	A 118		57.711	21.812	-0.952	1.00	23.50	A
	ATOM	377	CG2	ILE A	A 118		58.374	21.533	0.389	1.00	23.76	А
	ATOM	378	CG1	ILE A	A 118		56.246	21.362	-0.959	1.00	24.42	А
	ATOM	379	CD1	ILE 2	A 118		56.066	19.858	-0.834	1.00	28.06	· A
	ATOM	380	С	ILE 2	A 118		59.195	23.821	-0.958	1.00	23.78	A
10	ATOM	381	0	ILE 2	A 118		59.402	24.495	0.048	1.00	23.49	A
	ATOM	382	N	ILE 3	A 119		60.153	23.489	-1.815	1.00	23.46	A
	ATOM	383	CA		A 119		61.534	23.913	-1.619	1.00	25.13	A
	MOTA	384	CB		A 119		62.467	23.250	-2.664	1.00		A
	ATOM	385	CG2	ILE A			63.858	23.890	-2.617	1.00	22.47	A
15	ATOM	386	CG1				62.540	21.738	-2.395	1.00	25.05	A
	MOTA	387		ILE A			63.327	20.945	-3.439	1.00	24.62	Α
	MOTA	388	C̃		A 119		61.667	25.435	-1.705		25.96	A
	MOTA	389	0		A 119		62.330	26.051	-0.872	1.00	24.78	A
	MOTA	390	N		A 120		61.028	26.039	-2.704	1.00		A
20	MOTA	391	CA	LYS I		•	61.100	27.489	-2.879	1.00		А
	MOTA	392	СВ	LYS A			60.242	27.940	-4.060	1.00		A
	MOTA	393	CG	LYS A			60.674	27.407	-5.409	1.00		A
	ATOM	394	CD	LYS A			59.765	27.950	-6.512	1.00		A
0.7	MOTA	395	CE	LYS A			58.294	27.636	-6.218	1.00		A
25	MOTA	396	NZ	LYS A			57.363	28.155	-7.252	1.00		A
	ATOM	397	С	LYS A			60.647	28.247	-1.638		30.89	A
	MOTA	398	0		A 120.		61.303	29.198	-1.217	1.00		A
	ATOM	399	N	GLU Z			59.527	27.825	-1.055	1.00		A
30	ATOM	400	CA	GLU A			58.986	28.488	0.128	1.00		A
30	ATOM	401 402	CB	GLU A			57.455	28.416	0.117	1.00		A
	ATOM ATOM	402	CG CD	GLU A			56.794 57.221	29.021 30.456	-1.120 -1.373	1.00		A
	ATOM	404		GLU A			57.200	31.264	-0.420	1.00		A A
	ATOM	405		GLU A			57.573	30.778	-2.529	1.00		A
35	ATOM	406	C	GLU A			59.511	27.930	1.451	1.00		A
3.5	ATOM	407	0	GLU A			58.946	28.204	2.513	1.00		A
	ATOM	408	N	ASN A			60.588	27.151	1.390	1.00		A
	ATOM	409	CA	ASN A			61.183	26.573	2.594	1.00		A
•	ATOM	410	СВ	ASN A			61.836	27.673	3.436	1.00		A
40	ATOM	411	CG		122		62.945	28.395	2.698	1.00		A
	ATOM	412	OD1	ASN A			62.697	29.143	1.754	1.00		A
	ATOM	413		ASN A			64.181	28.169	3.127	1.00		A
	ATOM	414	С	ASN A	122		60.157	25.835	3.456	1.00	26.89	A
	ATOM	415	0	ASN A	122		60.085	26.055	4.663	1.00	27.23	A
45	ATOM	416 ·	N	LYS .	123		59.375	24.955	2.842	1.00	23.99	A
	ATOM	417	CA	LYS A			58.358	24.210	3.574	1.00		Α
	ATOM	418	CB	LYS F	123		57.031	24.248	2.810	1.00		A
	ATOM	419	CG	LYS F	123		56.475	25.645	2.599	1.00	25.68	A
	ATOM	420	CD	LYS F	123		56.253	26.354	3.927	1.00	27.54	A
50	MOTA	421	CE	LYS F	123		55.822	27.796	3.716	1.00	31.30	A
	MOTA	422	NZ	LYS F			55.756	28.540	5.004	1.00	33.21	A
	ATOM	423	C	LYS F			58.748	22.759	3.821	1.00	22.20	A
•	ATOM	424	0	LYS F			57.924	21.960	4.264	1.00		Α
	ATOM	425	N	VAL A			59.997	22.412	3.535	1.00		A
55	MOTA	426	CA	VAL A			60.439	21.039	3.730	1.00		Α
	MOTA	427	CB	VAL A			61.922	20.850	3.328	1.00		A
	MOTA	428		VAL A			62.346	19.407	3.573	1.00		Α
	MOTA	429		VAL A			62.104	21.195	1.853	1.00		Α
	ATOM	430	С	VAL A	124		60.236	20.561	5.163	1.00	19.53	A

	ATOM	431	0	VAL	A	124		59.841	19.418	5.385	1.00	20.02	A
	ATOM	432	N	PRO	A	125		60.513	21.422	6.159		20.01	A
	ATOM	433	CD	PRO					22.738	6.118			
								61.178				18.69	A
	ATOM	434	CA	PRO .				60.318	20.979	7.544	1.00	19.88	A
5	MOTA	435	CB	PRO .	A	125		60.793	22.180	8.363	1.00	19.95	A
	ATOM	436	CG	PRO .	Α	125		61.839	22.805	7.479		18.85	A
	ATOM	437	C	PRO .					20.642	7.824			
								58.848				19.76	A
	ATOM	438	0	PRO .	A	125		58.544	19.700	8.550	1.00	16.99	A
	ATOM	439	N	TYR .	A	126		57.947	21.418	7.235	1.00	18.98	A
10	MOTA	440	CA	TYR :	Α	126		56.516	21.220	7.435		21.97	A
	ATOM	441	CB										
				TYR .				55.752	22.448	6.933		25.17	A
	MOŢA	442	CG	TYR .				56.040	23.690	7.748	1.00	30.98	A
	ATOM .	443	CD1	TYR .	A :	126		55.438	23.886	8.991	1.00	33.95	A
	MOTA	444		TYR .				55.721	25.015	9.763	1.00	36.60	A
15	ATOM	445		TYR				56.938	24.657	7.292			
15												35.43	A
	ATOM	446	CE2	TYR .				57.231	25.792	8.058		37.20	A
,	ATOM	447	CZ	TYR .	A :	126		56.618	25.962	9.291	1.00	37.40	A
	ATOM	448	ОН	TYR .	Α :	126		56.903	27.073	10.052	1.00	40.85	A
	ATOM	449	С	TYR				55.990	19.956	6.762		21.35	A
20	MOTA	450	0	TYR I	Α.	126		55.265	19.175	7.383	1.00	20.49	A
	MOTA	451	N	VAL A	Α.	127		56.354	19.746	5.501	1.00	18.16	A
	ATOM	452	CA	VAL	Α :	127		55.892	18.562	4.790	1.00	17.58	Α
	ATOM	453	СВ	VAL				56.308	18.596	3.308		17.45	A
	MOTA	454		VAL 2				55.786	17.350	2.600		17.97	A
25	ATOM	455	CG2	VAL				55.751	19.850	2.641	1.00	14.90	А
	MOTA	456	С	VAL	Α :	127		56.459	17.306	5.448	1.00	18.39	A
	ATOM	457.	0	VAL	Α	127		55.769	16.298	5.583	1.00	18.14	A
	ATOM	458	N	THR				57.716	17.381	5.869		17.50	A
					-								
	MOTA	459	CA	THR I				58.375	16.260	6.530		18.54	A
30	MOTA	460	CB	THR I	A.	128		59.861	16.586	6.805	1.00	18.01	A
	ATOM	461	OG1	THR I	A :	128		60.537	16.804	5.559	1.00	21.14	A
	ATOM	462		THR				60.536	15.446	7.545		17.95	A
													A
	ATOM	463	С	THR				57.676	15.941	7.856		19.49	
	ATOM	464	0	THR I	Α.	128		57.438	14.776	8.179	1.00	18.76	A
35	ATOM	465	N	ARG A	Α :	129		57.345	16.981	8.619	1.00	19.60	А
	ATOM	466	CA	ARG I	Α .	129		56.673	16.804	9.904	1.00	20.12	A
	ATOM	467	СВ	ARG A				56.534	18.144	10.621		21.33	A
	ATOM	468	CG	ARG 2				55.948	18.029	12.023		28.02	A
	ATOM	469	CD	ARG A	Α.	129		55.721	19.404	12.597	1.00	31.25	A
40	ATOM	470	NE	ARG 2	Α :	129		56.940	20.205	12.560	1.00	37.78	A
	ATOM	471	CZ	ARG A				56.962	21.524	12.391	1.00	40.10	A
		•		ARG A				55.828	22.197	12.239		40.03	· A
	ATOM	472					-						
	ATOM	473	NH2	ARG 2				58.119	22.170	12.374		44.58	A
	MOTA	474	С	ARG A	A :	129		55.288	16.186	9.729		20.08	A
45	ATOM	475	0	ARG I	A :	129		54.891	15.305	10.496	1.00	20.40	A
	ATOM	476	N	GLU Z				54.553	16.654	8.724		18.79	A
	MOTA	477	CA	GLU A				53.222	16.125	8.454		20.10	A
	ATOM	478	CB	GLU A	4	130		52.638	16.749	7:183	1.00	19.92	A
	ATOM	479	CG	GLU A	Α :	130		51.350	16.087	6.708	1.00	27.85	A
50	ATOM	480	CD	GLU A				50.581	16.933	5.707	1.00	29.72	Α
				GLU A				51.216	17.528	4.814		33.46	, A
	ATOM	481											
	ATOM	482		GLU A				49.339	16.996	5.807		30.74	, A
	ATOM	483	С	GLU A		130		53.301	14.615	8.295		19.81	· A
	ATOM	484	0	GLU Z	4	130		52.553	13.875	8.935	1.00	18.37	A
55	ATOM	485	N	ARG I				54.219	14.162	7.447		20.41	A
				ARG A				54.397	12.735			22.45	A
	ATOM	486	CA							7.202			
	ATOM	487	CB	ARG A				55.442	12.511	6.098		25.16	A
	ATOM	488	CG	ARG 1		131		55.742	11.043	5.840	1.00	28.75	A
	ATOM	489	CD	ARG A	A :	131		56.736	10.837	4.708	1.00	33.75	· A
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	ATOM	490	NE	ARG	Α	131		57.020	9.	415	4.520	1.00	40.07	Α
	ATOM	491	CZ	ARG	Α	131		57.756	8.	915	3.532	1.00	43.07	A
	ATOM	492	NH1	ARG	A	131		58.293	9.	721	2.625		44.91	A
	ATOM	493	NH2	ARG	A	131		57.955	7.	606	3.449	1.00	44.45	A
5	MOTA	494	C	ARG	A	131		54.820	11.	982	8.466		23.24	A
	ATOM	495	0	ARG	A	131		54.241	10.	948	8.804		23.86	A
•	ATOM	496	N ·	ASP	Α	132		55.831	12.	497	9.160		21.99	A
	ATOM	497	CA	ASP	Α	132		56.318	11.	850	10.370		22.04	A
	ATOM	498	CB	ASP	Α	132		57.5 7 0	12.	564	10.888		23.72	A
10	ATOM	499	CG	ASP				58.750		442	9.932		27.77	Α
	MOTA	500		ASP				58.681	11.	620	8.989		27.34	Α
	MOTA	501	OD2	ASP	Α	132		59.753	13.	163	10.128		28.70	A
	ATOM	502	С	ASP	A	132		55.258	11.	772	11.474		21.69	A
	ATOM	503	0	ASP	Α	132		55.077		723	12.092		22.75	A
15	ATOM	504	N	VAL	Α	133		54.551		8 68	11.725		19.54	A
	ATOM	505	CA	VAL	A	133		53.525		843	12.759		18.52	A
	ATOM	506	CB	VAL	Α	133		52.908		244	12.990		19.26	Ą
	MOTA	507	CG1	VAL	A	133		51.708		135	13.918		18.79	A
	MOTA	508	CG2	VAL	A	133		53.953		180	13.604		18.80	A
20	ATOM	509	С	VAL	A	133		52.419		854	12.398		19.46	A
	MOTA	510	0	VAL	Α	133		52.073		991	13.200		19.94	Α,
	MOTA	511	N			134		51.878		957	11.187		19.15	A
	MOTA	512	CA			134		50.807		052	10.792		21.25	A
	MOTA	513	CB			134		50.309		381	9.383		17.34	. A
25	MOTA	514	CG			134		49.615		730	9.302		20.00	· A
	MOTA	515	SD			134		48.643		952	7.798		24.21	. A
	MOTA	516	CE			134		47.033		434	8.400		23.20	A A
	MOTA	517	C.			134		51.203		582	10.881		22.43	A
	MOTA	518	0			134		50.384		741	11.249		23.82 23.09	A
30	MOTA	519	N			135		52.454		273	10.556		26.13	A
	MOTA	520	CA			135		52.939		895	10.615		26.13	A
	MOTA	521	CB			135		54.356		.798	10.039 8.673		31.91	Α.
	MOTA	522	OG			135		54.383		.177	12.045		26.58	A
	ATOM	523	C			135		52.957		.358 .148	12.261		26.42	A
35	MOTA	524	0			135		52.926 53.014		. 261	13.018		25.65	A
	MOTA	525	N			136	•	53.014		. 201	14.425		27.47	A
	MOTA	. 526	CA			136		53.823		. 914	15.238		27.97	A
	MOTA	527	CB			136		55.283		.082	14.857		32.00	A
40	ATOM	528	CG			136		55.904		.218	15.664		33.03	A
40	ATOM	529	CD			136 136		55.602		.073	17.084		36.11	A
,	MOTA	530	NE			136		55.867		.990	18.007		39.74	A
	MOTA	531	CZ	ARG ARG				56.449		.132	17.661		40.55	. A
	ATOM	532 533		ARG				55.540		.769	19.276		36.72	A
45	MOTA					136		51.667		.709	15.036		26.38	A
45	MOTA	534	С 0			136		51.516		.121	16.106		27.06	A
	ATOM ATOM	535 536	N	TEI	Δ	137		50.655		.235	14.360		24.77	' A
	ATOM	537	CA			137		49.294		.162	14.870		24.70	A
	ATOM	538	CB			137		48.483		. 363	14.371		24.52	· A
50	ATOM	539	CG			137		49.050		.760	14.662		26.67	A
30	ATOM	540		LEU				48.075		.813	14.141	1.00	27.25	A
	ATOM	541		LEU				49.279		. 945	16.155	1.00	27.09	A
	ATOM	542	C			137		48.592		.868	14,473	1.00	25.20	A
	ATOM	543	Õ			137		48.619		.469	13.309		25.99	A
55	ATOM	544	N			138		47.971		.218	15.451		21.89	A
55	ATOM	545	CA			138		47.239		. 977	15.219		21.35	A
	ATOM	546	СВ			138		48.124		.761	15.523		22.14	A
	ATOM	547	CG			138		47.432		.448	15.201		24.90	
	ATOM	548				138		46.631		.423	14.241	1.00	24.78	A

	ATOM	549	OD2	ASP	Α	138		47.691	1.443	15.897	1.00 25.39	A
	ATOM	550	С			138		46.031	4.991	16.138	1.00 20.47	A
	ATOM	551	Ō			138	•	45.967	4.248	17.118	1.00 19.06	A
	ATOM	552	N			139		45.075	5.852	15.810	1.00 18.27	A
5	ATOM	553	CA			139		43.869	6.016	16.606	1.00 18.21	A
•	ATOM	554	СВ			139		44.096	7.157	17.612	1.00 15.84	A
•		555	CG			139		42.985	7.332	18.600		
	ATOM			HIS					6.964		1.00 15.24	,A
	MOTA	556						42.884		19.900	1.00 13.97	A
10	ATOM	557		HIS				41.791	7.943	18.280	1.00 14.74	A
10	ATOM	558		HIS				41.002	7.944	19.341	1.00 14.19	A
	ATOM	559		HIS				41.641	7.356	20.336	1.00 14.15	A
	ATOM	560	C	HIS				42.715	6.330	15.654	1.00 18.50	A
	MOTA	561	0	HIS				42.879	7.080	14.693	1.00 20.80	A
	MOTA	562	N	PRO	Α	140		41.527	5.767	15.913	1.00 18.32	A
15	ATOM	563	CD	PRO				41.143	4.984	17.100	1.00 16.71	A
	ATOM	564	CA	PRO	Α	140		40.367	6.001	15.048	1.00 17.43	A
	ATOM	565	CB	PRO	А	140		39.273	5.157	15.704	1.00 16.64	Α
	ATOM	566	CG	PRO	Α	140		39.643	5.204	17.152	1.00 18.43	A
	ATOM	567	С	PRO	Α	140		39.914	7.441	14.803	1.00 18.77	A
20	ATOM	568	0	PRO	A	140		39.207	7.695	13.831	1.00 19.88	A
	ATOM	569	N	PHE				40.301	8.381	15.664	1.00 17.14	A
	ATOM	570	CA	PHE	А	141		39.874	9.767	15.477	1.00 16.42	А
	ATOM	571	CB	PHE				39.568	10.422	16.836	1.00 14.60	А
	ATOM	572	CG	PHE				38.386	9.817	17.556	1.00 15.26	A
25	ATOM	573		PHE				37.335	9.234	16.842	1.00 14.78	A
23	ATOM	574		PHE				38.297	9.880	18.942	1.00 13.70	A
	ATOM	575		PHE				36.215	8.727	17.502	1.00 16.94	A
	ATOM	576		PHE				37.178	9.375	19.615	1.00 15.75	A
	ATOM	577	CZ	PHE				36.135	8.799	18.893	1.00 16.89	A
20			C					40.857	10.641	14.694	1.00 16.15	A
30	ATOM	578 570		PHE				40.837	11.871	14.054	1.00 10.15	Ā
	ATOM	579	0 .	PHE							1.00 17.33	A
	ATOM	580	N	PHE				41.748	10.011	13.941		A
	ATOM	581	CA	PHE				42.727	10.756	13.154	1.00 17.89	
	MOTA	582	CB	PHE				44.115	10.645	13.793	1.00 17.57	A
35	MOTA	583	CG	PHE				44.240	11.371	15.103	1.00 18.74	A
	ATOM'	584		PHE				44.559	12.726	15.135	1.00 17.77	A
	ATOM	.585		PHE				43.997	10.711	16.304	1.00 18.74	A
	MOTA	586		PHE				44.632	13.417	16.347	1.00 15.77	A
	ATOM	587		PHE	-			44.065	11.393	17.522	1.00 17.56	A
40	ATOM	588	CZ	PHE				44.383	12.747	17.542	1.00 17.14	A
	MOTA	589	С	PHE				42.793	10.231	11.729	1.00 19.12	A
	MOTA	590	0	PHE	Α	142		42.659	9.030	11.504	1.00 20.01	A
	ATOM	591	N	VAL	A	143		42.978	11.135	10.769	1.00 18.72	Α
	ATOM	592	CA	VAL	Α	143		43.102	10.735	9.371	1.00 18.52	A
45	MOTA	593	CB	VAL	Α	143		43.294	11.961	8.440	1.00 20.66	A
	ATOM	594	CG1	VAL	A	143		43.843	11.521	7.080	1.00 21.29	A
	ATOM	595	CG2	VAL	Α	143		41.958	12.673	8.252	1.00 22.97	Α
	ATOM	596	С	VAL	Α	143		44.342	9.865	9.330	1.00 18.68	A
	ATOM	597	0	VAL	Α	143		45.355	10.199	9.943	1.00 18.42	· A
50	ATOM	598	N	LYS				44.259	8.745	8.623	1.00 18.30	A
	ATOM	599	CA	LYS				45.384	7.824	8.535	1.00 18.78	` A
	ATOM	600 .		LYS				44.889	6.373	8.608	1.00 22.27	Α
	ATOM	601	CG	LYS				46.017	5.340	8.557	1.00 29.72	. A
	ATOM	602	CD	LYS				45.491	3.912	8.674	1.00 34.16	A
55	ATOM	603	CE	LYS				46.631	2.896	8.577	1.00 37.67	A
در	ATOM	604	NZ	LYS				46.138	1.484	8.629	1.00 37.07	A
	ATOM	605	C	LYS				46.192	8.002	7.261	1.00 33.02	A
		606	0	LYS				45.643	8:314	6.200	1.00 18.33	A
	ATOM										1.00 16.18	A
	MOTA	607	N	LEU	H	TAO		47.502	7.816	7.385	1.00 IU./3	A

	ATOM	608	CA	LEU · F	145	48.411	7.900	6.251	1.00 17.45	A
	ATOM	609	CB ·	LEU F	145	49.686	8.653	6.641	1.00 18.82	Α
	ATOM	610	CG	LEU F	145	50.734	8.902	5.549	1.00 20.23	A
	ATOM	611	CD1	LEU A	145	51.836	9.799	6.093	1.00 18.83	A
5	ATOM	612	CD2	LEU F	145	51.317	7.581	5.069	1.00 19.79	Α
	MOTA	613	С	LEU P	145	48.739	6.450	5.907	1.00 19.19	Α
	MOTA	614	0	LEU F	145	49.451	5.772	6.659	1.00 17.36	A
•	ATOM	615	N	TYR F	146	48.215	·· 5.972	4.782	1.00 17.28	Α
	ATOM	616	CA	TYR F	146	48.444	4.593	4.358	1.00 17.57	A
10	ATOM	617	СВ	TYR F	146	47.288	4.098	3.486	1.00 17.74	, A
	ATOM	618	CG	TYR F	146	45.981	3.926	4.214	1.00 17.50	Α
٠.	ATOM	619	CD1	TYR P	146	45.099	4.995	4.377	1.00 16.50	Α
	ATOM	620	CE1	TYR F	146	43.881	4.827	5.039	1.00 17.10	A
	ATOM	621	CD2	TYR F	146	45.620	2.686	4.735	1.00 18.28	A
15	ATOM	622	CE2	TYR F	146	44.411	2.506	5.399	1.00 19.84	Α
	ATOM	623	CZ	TYR F	146	43.547	3.576	5.544	1.00 17.53	A
	ATOM	. 624	OH	TYR F	146	42.342	3.376	6.169	1.00 20.67	A
	MOTA	625	С	TYR F	146	49.735	4.376	3.582	1.00 18.72	A
	ATOM	626	0	TYR F	146	50.382	3.338	3.715	1.00 19.51	Α
20	ATOM	627	N	PHE F	147	50.110	5.350	2.765	1.00 18.09	A
	MOTA	628	CA	PHE F	147	51.307	5.203	1.952	1.00 17.20	A
	MOTA	629	СВ	PHE A	147	51.007	4.258	0.783	1.00 16.77	Α
	ATOM	630	CG	PHE A	147	49.835	4.699	-0.070	1.00 17.75	A
	ATOM	631	CD1	PHE A	147	49.967	5.752	-0.975	1.00 16.58	A
25	MOTA	632	CD2	PHE F	147	48.595	4.075	0.053	1.00 18.07	A
	ATOM	633	CE1	PHE A	147	48.886	6.178	-1.742	1.00 19.62	A
	ATOM	634	CE2	PHE A	147	47.503	4.492	-0.710	1.00 18.56	A
	MOTA	635	CZ	PHE A	147	47.647	5.546	-1.610	1.00 19.27	A
	MOTA	636	С	PHE A	147	51.768	6.533	1.395	1.00 17.13	A
30	MOTA	637	0	PHE A	147	51.045	7.528	1.452	1.00 14.43	A
	ATOM	638	N	THR F	148	52.981	6.534	0.854	1.00 17.12	Α
	ATOM	639	CA	THR A	148	53.541	7.718	0.232	1.00 17.96	A
	MOTA	640	CB.	THR A	148	54.449	8.531	1.197	1.00 21.51	A
	MOTA	641	OG1	THR A	148	55.605	7.760	1.537	1.00 18.83	A
35	MOTA	642	CG2	THR A	148	53.700	8.897	2.472	1.00 19.60	A
	MOTA	643	C	THR A	148	54.386	7.262	-0.946	1.00 20.31	A
	ATOM	644	0	THR A	148	54.860	6.124	-0.991	1.00 18.94	Α
	MOTA	645	N	PHE A	149	54.543	8.149	-1.916	1.00 19.16	Α
	MOTA	646	CA	PHE A	149	55.368	7.877	-3.073	1.00 18.01	A
40	MOTA	647	CB	PHE A	149	54.748	6.801	-3.989	1.00 17.23	A
	MOTA	648	CG	PHE A	149	53.389	7.144	-4.544	1.00 16.88	Α
	ATOM	649	CD1	PHE A	149	53.262	7.888	-5.712	1.00 18.58	Α
	ATOM	650	CD2	PHE A	149	52.235	6.668	-3.927	1.00 17.31	A
	ATOM	651	CE1	PHE A	A 149	52.007	8.149	-6.267	1.00 19.26	A
45	ATOM	652	CE2	PHE A	A 149	50.972	6.923	-4.470	1.00 19.17	. A
	MOTA	653	CZ	PHE A	149	50.858		-5.642	1.00 19.60	A
	ATOM	654	С	PHE A	149	55.542	9.205	-3.774	1.00 20.85	Α
	ATOM	655	0	PHE A	149	54.934	10.200	-3.376	1.00 19.76	A
	ATOM	656	N	GLN A		56.398	9.241	-4.782	1.00 19.79	A
50	MOTA	657	CA	GLN A	150	56.636	10.481	-5.497	1.00 24.03	Α
	ATOM	658	CB	GLN A		57.659	11.347	-4.739	1.00 24.45	A
	MOTA	659	CG	GLN A		58.986	10.645	-4.414	1.00 26.28	A
	MOTA	660	CD	GLN A		59.988	11.558	-3.692	1.00 29.02	A
	MOTA	661	OE1	GLN A		60.693	12.353	-4.321	1.00 27.05	A
55	MOTA	662	NE2			60.042	11.449	-2.365	1.00 26.47	A
	MOTA	663	С	GLN A		57.160	10.203	-6.885	1.00 23.88	A
	MOTA	664	0	GLN A		57.673	9.118	-7.158	1.00 24.79	A
	MOTA	665	N	ASP A		56.987	11.171	-7.774	1.00 25.88	A
	MOTA	666	CA	ASP 1	A 151	57.527	11.047	-9.117	1.00 26.49	A

	T. (10.) 4	667	an.			56 437	11 100	10 100				
•	MOTA	667	СВ		A 151			-10.199		24.54	A	
	ATOM	668	CG		A 151	55.544		~10.064		24.95	A	
	MOTA	669			A 151	56.005	13.379	-9.561		22.44	A	
	ATOM	670	OD2	ASP	A 151	54.369	12.242	-10.490	1.00	25.72	A	
5	ATOM	671	С	ASP	A 151	58.515	12.203	-9.220	1.00	28.63	A	
	ATOM	672	0	ASP	A 151	58.890	12.780	-8.194	1.00	27.83	A	
	ATOM	.673	N	ASP	A 152	58.934	12.560	-10.426		29.21	A	
	ATOM	674	CA		A 152	59.907	13.636	-10.562		31.88	A	
	ATOM	675	CB		A 152	60.325		-12.026		33.94	A	
10	ATOM	676	CG		A 152	61.033		-12.557		38.88	A	
10	ATOM	677						-11.791		39.67		
					A 152	61.817					A	
	ATOM	678			A 152	60.817		-13.738		41.57	A	
	MOTA	679	С		A 152	59.487		-10.013		30.90	A	
	ATOM	680	0		A 152	60.316	15.735	-9.482		31.69	A	
15	ATOM	681	N		A 153	58.207		-10.107		29.44	A	
	ATOM	682	CA	GLU .	A 153	57.767	16.632	-9.646	1.00	28.69	A	
	ATOM	683	CB	GLU .	A 153	56.984	17.327	-10.766	1.00	32.90	A	
	ATOM	684	CG	GLU .	A 153	57.451	16.987	-12.183	1.00	40.57	· A	
	ATOM	685	CD	GLU .	A 153	56.920	15.643	-12.675	1.00	45.78	A	
20	ATOM	686	OE1	GLU .	A 153	55.682	15.482	-12.760	1.00	48.91	A	
	ATOM	687			A 153	57.736		-12.979		48.95	A	
	ATOM	688	C		A 153	56.929	16.683	-8.372		26.43	A	
	ATOM	689	Ö		A 153	56.947	17.688	~7.660		25.08	A	
	ATOM	690	N.		A 154	56.205	15.610	-8.069		22.39	A	
25		691			A 154	55.318	15.631			21.43	A	
23	ATOM		CA									
	ATOM	692	CB		A 154	53.861	15.628	-7.398		20.33	A	
	MOTA	693	CG		A 154	53.505	16.716	-8.403		21.92	A	
	MOTA	694	CD		A 154	52.211	16.375	-9.146		19.70	A	
	MOTA	695	CE		A 154	51.775		-10.077		20.04	A	
30	ATOM	696	NZ		A 154	50.631		-10.951		19.97	A	
	ATOM	697	С	LYS .	A 154	55.458	14.522	-5.881		20.43	A	
	ATOM	698	0	LYS .	A 154	55.949	13.426	-6.173	1.00	21.13	A	
	. ATOM	699	N	LEU .	A 155	54.985	14.832	-4.676	1.00	19.69	A	
	ATOM	700	CA	LEU .	A 155	54,950	13.900	-3.553	1.00	19.10	A	
35	ATOM	701	CB	LEU .	A 155	55.362	14.588	-2.252	1.00	19.65	A	
	ATOM	702	CG	LEU .	A 155	56.740	15.234	-2.129	1.00	21.20	A	
	ATOM	703			A 155	56.848	15.918	-0.770	1.00	23.42	А	
	ATOM	704			A 155	57.816	14.174	-2.277		23.08	, A	
	ATOM	705	C		A 155	53.478	13.507	-3.427		18.87	A	
40	ATOM	706	Ö		A 155	52.600	14.348	-3.620		18.61	A	
40	ATOM	707	Ŋ		A 156	53.209	12.249	-3.091		15.02	A	
		707			A 156	51.834	11.783	-2.934		16.29	A	
	ATOM		CA			51.470	10.769	-4.029		14.20	A	
	ATOM	709	CB		A 156							
	ATOM	710	CG		A 156	51.603	11.273	-5.449		17.29	A	
45	ATOM	711			A 156			-6.045		16.46	A	
	ATOM	712			A 156	52.978	11.884	-7.360		18.68	A	
	ATOM	713			A 156	50.474	11.588	-6.202		16.43	Α	
	ATOM	714	CE2	TYR .	A 156	50.583	12.048	-7.512	1.00	16.31	Α	
	ATOM	715	CZ	TYR .	A 156	51.835	12.192	-8.083	1.00	18.17	Α	
50	ATOM	716	OH	TYR .	A 156	51.941	12.651	-9.371	1.00	17.47	A	
	ATOM	717	С	TYR .	A 156	51.657	11.108	-1.572	1.00	16.32	A	
	ATOM	718	0		A 156	52.412	10.197	-1.235		16.27	A	
	ATOM	719	N		A 157	50.678	11.568	-0.792		15.47	A	
	ATOM	720	CA		A 157	50.385	10.966	0.508		16.66	A	
55	ATOM	721	CB		A 157	50.324	12.014	1.629		16.91	A	
J.J	ATOM	721	CG		A 157	51.631	12.708	1.907		18.96	A	
						52.821	12.766	1.340		20.31	A	
	ATOM	723			A 157	51.664	13.829	2.732		21.12	A	
	ATOM	724			A 157					22.08		
	ATOM	725	CLI	PHE 2	7 T2/	54.025	12.926	1.585	1.00	24.08	A	

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_	ATOM	726	CE2	PHE A	157	52.865	14.500	2.982	1.00	22.18	Α
•	ATOM	727	CZ	PHE A	157	54.045	14.045	2.405	1.00	21.27	A
		728	C	PHE A		49.016	10.308	0.404		16.52	A
	ATOM										
• .	MOTA	729	Ö	PHE A		48.029	10.979	0.110		17.32	A
5	ATOM	730	N	GLY A	158	48.953	9.002	0.644	1.00	15.97	A
	MOTA	731	CA	GLY A	158	47.684	8.299	0.572	1.00	16.13	A
	ATOM	732	С	GLY A	158	47.000	8.383	1.920	1.00	14.94	A
		733		GLY A		47.445	7.756	2.879		16.28	A
	ATOM		0								
	ATOM	734	N	LEU A		45.915	9.145	1.989		13.50	A
10	MOTA	735	CA	LEU A	159	45.191	9.340	3.241		15.20	A
	ATOM	736	CB	LEU A	159	45.031	10.835	3.517	1.00	14.20	Α
	ATOM	737	CG	LEU A	159	46.270	11.726	3.385	1.00	19.00	A
	ATOM	738		LEU A		45.847	13.188	3.477	1.00	17.12	A
				LEU A		47.275	11.390	4.471		14.71	A
	ATOM	739								15.53	A
15	ATOM	740	С	LEU A		43.809	8.716	3.232			
	ATOM	741	0	LEU A		43.232	8.472	2.177		16.05	A
	ATOM	742	N	SER A	160	43.268	8.469	4.418	1.00	15.86	A
	ATOM	743	CA	SER A	160	41.932	7.917	4.498	1.00	19.01	A
	ATOM	744	СВ	SER A		41.566	7.582	5.949	1.00	22.90	A
20		745	OG	SER A		41.901	8.629	6.833		24.18	A
20	MOTA						8.968	3.924		20.43	A
	MOTA	746	С	SER A		40.987					
	MOTA	747	0	SER A		41.213	10.173	4.062		19.96	A
	ATOM	748	N	TYR A	161	39.945	8.508	3.250		19.20	A
	MOTA	749	CA	TYR A	161	38.975	9.406	2.644	1.00	20.37	Α
25	MOTA	750	СВ	TYR A	161	38.471	8.785	1.332	1.00	20.00	A
23		751:	CG	TYR A		37.314	9.502	0.666	1.00	20.72	A
	AŢOM					37.222	10.895	0.682		18.22	A
	MOTA	752		TYR A			11.557	0.029		22.24	A
	MOTA	753		TYR P		36.180					
	MOTA	754	CD2	TYR A	. 161	36.333	8.784	-0.020		20.53	A
30	ATOM	755	CE2	TYR A	161	35.287	9.436	-0.678		24.24	Α.
	ATOM	756	CZ	TYR A	161	35.218	10.822	-0.648	1.00	22.32	A
	ATOM	757	ОН	TYR A	161	34.194	11.471	-1.298	1.00	23.03	A
	ATOM	758	C	TYR F		37.812	9.681	3.598	1.00	20.14	A
						36.959	8.819	3.810		19.53	A
	ATOM	759	0	TYR F				4.178		19.92	A
35	ATOM	760	N	ALA F		37.791	10.880				
	MOTA	761	CA	ALA A	162	36.721	11.271	5.099		21.07	A
	ATOM	762	CB	ALA '	162	37.187	12.419	6.002		19.60	, A
	ATOM	763	С	ALA A	162	35.542	11.712	4.238	1.00	22.07	A
	ATOM	764	Ō	ALA A		35.436	12.875	3.860	1.00	20.66	A
40	ATOM	765	N	LYS F		34.653	10.769	3.945	1.00	23.27	A
40		,		LYS F		33.503	11.017	3.080		27.12	. A
	ATOM	766	CA				9.741	2.963		29.68	A
	ATOM	767	CB	LYS F		32.663				37.67	A
	ATOM	768	CG	LYS F		33.455	8.524	2.515			
	ATOM	769	CD	LYS A	163	32.556	7.310	2.321		42.24	A
45 .	ATOM	770	CE	LYS F	163	33.373	6.034	2.185	1.00	44.48	A
	ATOM	771	NZ	LYS F		34.143	5.735	3.430	1.00	44.88	A
	ATOM	772	C	LYS A		32.581	12.186	3.411	1.00	25.78	A
						32.103	12.863	2.506		26.53	A
	ATOM	773	0	LYS 7						24.57	A
	MOTA	774	N	ASN A		32.327	12.441	4.689			
50	MOTA	775	CA	ASN A	164	31.420	13.522	5.033		23.77	A
	MOŤA	776	CB	ASN A	164	30.610	13.129	6.265	1.00	25.02	A
	ATOM	777	CG	ASN A	164	29.537	12.101	5.932	1.00	27.54	A
	MOTA	778		ASN A		28.772	12.281	4.983	1.00	28.79	A
				ASN A		29.475	11.024	6.704		27.13	A
	ATOM	779				31.999	14.931	5.169		24.43	A
55	ATOM	780	C	ASN A							
	ATOM	781	0	ASN A		31.306	15.856	5.589		23.98	A
	ATOM	782	N	GLY A	165	33.262	15.097	4.795		21.56	A
	ATOM	783	CA	GLY A		33.873	16.414	4.836		24.39	A
	MOTA	784	С	GLY A		34.191	17.043	6.181	1.00	23.62	A

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	ATOM	785	0.	SLY A	165		34.380	16.352	7.177	1.00 2	23.26	· A
		786			166		34.234	18.373	6.186	1.00 2	23.22	A
	ATOM	787		SLU A			34.563	19.176	7.362	1.00 2		A
	ATOM			SLU A			35.055	20.558	6.913	1.00 2		A
_	MOTA	788			166		36.419	20.569	6.229	1.00 2		A
5	ATOM	789					36.699	21.889	5,517	1.00		A
	MOTA	790			166			22.906	5.889		29.33	A
	ATOM	791	OE1				36.081			1.00		A
	ATOM	792			166		37.544	21.916	4.596			A
	ATOM	793	-		166		33.436		8.369	1.00		A
10	ATOM	794	_		166		32.279	19.541	8.001	1.00		
	ATOM	795			167		33.791	19.370	9.649	1.00		A
	MOTA	796	CA I	LEU F	167		32.813	19.581	10.707	1.00		A
	ATOM	797	CB I	LEU F	167		33.497	19.481	12.073	1.00		A
	ATOM	798	CG I	LEU <i>F</i>	167		32.706	19.923	13.306	1.00		A
15	ATOM	799	CD1	LEU A	167		31.454	19.074	13.463	1.00		A
13	ATOM	800			167		33.597	19.805	14.537	1.00		A
	ATOM	801			167		32.193	20.971	10.529		23.49	A
	ATOM	802			167		31.047	21.209	10.907	1.00	23.56	A
		803	_		1 168		32.960	21.887	9.948	1.00	24.25	Α
00	MOTA	804			1 168		32.473	23.245	.9.722	1.00	26.64	A
20	ATOM				1 168		33.560	24.099	9.066	1.00		A
	MOTA	805			A 168		33.198	25.546	8.707	1.00		A
•	MOTA	806			A 168		32.718	26.296	9.946		26.42	A
	MOTA	807					34.418	26.238	8.119		26.74	A
	ATOM	808			A 168		31.234	23.218	8.829		27.13	Α
25·	•	809			A 168			23.210	9.030		26.01	A
	MOTA	810			A 168		30.297		7.848		26.41	A
	MOTA	811			A 169		31.233	22.320	6.934		27.70	A
	MOTA	812			A 169		30.106	22.210			30.49	A
	MOTA	813			A 169		30.324	21.064	5.945		32.47	A
30	MOTA	814			A 169		29.151	20.854	4.993			A
	MOTA	815			A 169		29.407	19.728	3.998		35.98	A
	MOTA	816	CE	LYS .	A 169		29.462	18.372	4.683		38.53	A
	ATOM	817			A 169		29.622	17.263	3.702		41.00	
	ATOM	818			A 169		28.801	21.985	7.682		28.12	A
35	ATOM	819	0	LYS .	A 169		27.785	22.608	7.371		28.08	A
	ATOM	820	N	TYR .	A 170		28.826	21.094	8.668		26.53	A
	ATOM	821	CA	TYR .	A 170		27.624	20.791			26.95	A
	ATOM	822	CB		A 170		27.810	19.476	10.193		25.03	A
	MOTA	823	CG	TYR	A 170		27.898	18.300	9.251		26.65	A
40	ATOM	824			A 170		26.745	17.661	8.790		28.27	A
40	ATOM	825			A 170		26.814	16.642	7.839		26.85	A
	ATOM	826			A 170		29.127	17.884	8.742		27.83	A
	ATOM	827			A 170		29.209	16.869	7.792		27.19	A
*		828	CZ		A 170		28.049	16.254	7.343	1.00	30.02	A
4.5	ATOM	829	OH		A 170			15.268	6.382	1.00	29.23	Α
45	ATOM		C .		A 170		27.229	21.918	10.376		27.59	A
	ATOM	830					26.045	22.122	10.642		29.25	A
	ATOM	831	0		A 170 A 171		28.208	22.660	10.882		28.16	. A
	ATOM	832	N				27.883	23.770	11.763		29.03	A
	ATOM	833	CA		A 171		29.151	24.435	12.337		27.51	A
50	MOTA	834	CB		A 171				13.084		27.97	A
	ATOM	835			A 171		28.773	25.705	13.272		26.70	A
	ATOM	836			A 171		29.872	23.458	13.856		24.07	A
	MOTA	837			A 171		31.163	23.996			31.41	A
	MOTA	838	С		A 171		27.094	24.796	10.944		31.69	A
55	ATOM	839	0		A 171		26.088	25.335	11.407		33.21	A
•	MOTA	840	N		A 172		27.546	25.047	9.719			A
	ATOM	841	CA		A 172		26.874	26.000	8.844		36.54	
	MOTA	842	CB		A 172		27.734	26.314			37.73	A 7
	ATOM	843	CG	ARG	A 172	:	29.057	27.011	7.912	1.00	41.65	A

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	ATOM	844	CD	ARG	Α	172		29.708	27.492	6.616	1.00	45.29		A
	ATOM		NE	ARG				31.037	28.070	6.812		48.51		A ·
		846	CZ	ARG				31.314	29.059	7.658		51.53		A
	ATOM					_								
	ATOM	847		ARG				30.355	29.593	8.406		53.75		A
5	MOTA	848	NH2	ARG				32.553	29.526	7.748		51.21		A
	ATOM	849	С	ARG	Α	172		25.528	25.459	8.378	1.00	37.67		Α
•	ATOM	850	0	ARG	Α	172		24.550	26.200	8.288	1.00	39.09		A
	ATOM	851	N	LYS	Α	173		25.481	24.163	8.092	1.00	38.44		A
	ATOM	852	CA	LYS				24.259	23.528	7.619		39.25		A
10	ATOM	853	CB.	LYS				24.523	22.061	7.272		41.89		A
10									21.298	6.830		45.52		A
	ATOM	854	CG	LYS				23.279		_				
	ATOM	855	CD			173		23.557	19.808	6.653		49.60		Α ΄
	ATOM	856	CE	LYS	A	173		24.477	19.530	5.469		52.63		A
	ATOM	857	NZ	LYS	Α	173		23.855	19.894	4.160	1.00	54.61		Α
15	ATOM	858	C·	LYS	Α	173		23.089	23,608	8.595	1.00	39.30		Α
	ATOM	859	0	LYS				21.981	23.960	8.201	1.00	39'.62		Α
	ATOM	860	N	ILE				23.320	23.282	9.863		37.96		A
		861		ILE				22.229	23.314	10.833		37.36		A
	ATOM		CA											
	MOTA	862	CB	ILE				22.159	21.998	11.652		37.44		A
20	ATOM	863		ILE			•	22.058	20.802	10.709		38.37		Α
	ATOM	864	CG1	ILE	A	174		23.397	21.850	12.532	1.00	37.25		A
	ATOM	865	CD1	ILE	Α	174		23.355	20.620	13.418	1.00	36.85		Α
	, ATOM	866	C ·	ILE	Α	174		22.259	24.492	11.801	1.00	36.71		Α
	ATOM	867	Ō	ILE				21.448	24.556	12.724		38.05		A
25	ATOM	868	N			175		23.185	25.423	11.592		35.48		Ā
25									26.585	12.462		35.29		A
	MOTA	869	CA	GLY				23.265						
	ATOM	870	С			175		24.053	26.360	13.737		35.06		A
	ATOM	871	0	GLY	Α	175		25.066	27.019	13.970		37.46		Α
	MOTA	872	N	SER	Α	176		23.581	25.441	14.571	1.00	33.94		Α
30	ATOM	873	CA	SER	Α	176		24.253	25.113	15.822	1.00	32.84		Α
	ATOM	874	CB			176		23.938	26.155	16.901	1.00	33.54		Α
	ATOM	875	OG	SER				22.599	26.056	17.347	1.00	34.86		Α
	ATOM	876	C			176		23.796	23.731	16.276		32.34		Α
						176		22.726	23.263	15.884		32.82		A
à	ATOM	877	0									29.39		Α
35	MOTA	. 878	N			177		24.609	23.085	17.103				
	MOTA	879	CA			177		24.313	21.743	17.597		27.20		A
	MOTA	880	CB	PHE	Α	177		25.621	20.989	17.865		26.39		A
	ATOM	881	CG	PHE	Α	177		26.372	20.585	16.622	1.00	26.18		A
	ATOM	882	CD1	PHE	Α	177		26.210	21.277	15.426	1.00	25.30		A
40	ATOM	883	CD2	PHE	Α	177		27.266	19.516	16.662	1.00	26.05		Α
	ATOM	884		PHE				26.923	20.912	14.290		26.59		Α
	ATOM	885		PHE				27.986	19.143	15.532		26.06		A
								27.815	19.841	14.343		25.42		A
	ATOM	886	CZ			177								
	ATOM	887	С	PHE				23.500	21.752	18.884		27.00		A
45	ATOM	888	0	PHE				23.704		19.747		26.48		A
	ATOM	889	N	ASP	Α	178		22.578	20.802	19.022		26.70		Α
	ATOM	890	CA	ASP	Α	178		21.816	20.729	20.260	1.00	26.35		Α
	ATOM	891	CB	ASP				20.621	19.773	20.142	1.00	29.90		A
	ATOM	892	CG	ASP				21.020	18.372	19.720		32.28		A
50		893		ASP				22.157	17.949	20.014		35.21		A
20	ATOM											34.79		A
	ATOM	894		ASP				20.179	17.683	19.105				
	ATOM	895	С	ASP				22.810	20.228	21.311		25.03		A
	ATOM	896	0	ASP				23.974	19.968	20.992		21.24		Α.
	MOTA	897	N	GLU	Α	179		22.361	20.083	22.552		23.60		Α
55	ATOM	898	CA	GLU	Α	179		23.247	19.644	23.619		25.18	-	A
	ATOM	899	CB	GLU	Α	179		22.542	19.770	24.971	1.00	27.60		Α
	ATOM	900		GLU				23.324	19.176	26.130		32.58		Α -
•	ATOM	901	CD	GLU				22.997	19.845	27.449		35.82		A
		902		GLU				21.825	20.224	27.645		35.95		A
	ATOM	302	OET	GTO	H	113		21.023	40.44	21.043	1.00	22.23		••

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	ATOM	903	OE2	GLU	A	179		23.912	19.984	28.291	1.00	38.19	A
	ATOM	904	С	GLU	A	179		23.808	18.235,	23.450	1.00	24.08	Ā
	ATOM	905	0	GLU	A	179		24.977	17.989	23.756	1.00	22.79	Α
	MOTA	906	N	THR	Α	180		22.983	17.316	22.961	1.00	23.36	A
5	ATOM	907	CA	THR	Α	180		23.412	15.935	22.761	1.00	22.15	A
	ATOM	908	CB	THR	Α	180		22.224	15.054	22.320	1.00	23.77	A
	ATOM	909		THR				21.222	15.075	23.341	1.00	26.37	A
	ATOM	910	CG2	THR	Α	180		22.670	13.616	22.088	1.00	22.66	А
	ATOM	911	С	THR	Α	180		24.533	15.830	21.724	1.00	22.01	A
10	ATOM	912	0	THR	Α	180		25.533	15.141	21.944	1.00	19.87	A
	ATOM	913	N	CYS	Α	181		24.365	16.511	20.596	1.00	21.21	A
	ATOM .	914	CA	CYS	Α	181		25.372	16.480	19.541	1.00	22.22	A
	ATOM	915	CB	CYS	Α	181		24.800	17.065	18.250	1.00	24.62	A
	ATOM -	916	SG	CYS	Α	181		23.435	16.080	17.560	1.00	29.50	A
15	ATOM	917	С	CYS	Α	181		26.633	17.232	19.954	1.00	23.07	A
	ATOM	918	0	CYS	Α	181		27.746	16.827	19.608	1.00	23.95	A
	ATOM	919	N	THR	Α	182		26.463	18.325	20.695	1.00	22.76	A
	ATOM	920	CA	THR	Α	182		27.606	19.103	21.161	1.00	21.49	A
	ATOM	921	CB	THR	Α	182		27.167	20.346	21.978	1.00	21.37	A
20	ATOM	922	OG1	THR	A	182		26.459	21.262	21.134	1.00	22.50	A
	ATOM	923	CG2	THR	Α	182	•	28.379	21.046	22.565	1.00	18.36	A
	ATOM	924	C	THR	A	182		28.454	18.215	22.071	1.00	21.48	A
	MOTA	925	0	THR	Α	182		29.669	18.090	21.894	1.00	19.95	A
	ATOM	926	N	ARG	Α	183		27.798	17.602	23.050	1.00	18.97	A
25	MOTA	927	CA	ARG	А	183		28.468	16.723	23.996	1.00	19.39	A
	MOTA	928	CB	ARG	A	183		27.455	16.140	24.984	1.00	19.46	A
	ATOM	929	CG	ARG	Α	183		28.030	15.062	25.887	1.00	18.77	Α
	ATOM	930	CD	ARG	Α	183		27.021	14.571	26.925	1.00	21.19	A
	ATOM	931	NE	ARG	A	183		26.605	15.642	27.824	1.00	19:46	A
30	ATOM	932	CZ	ARG	A	183		25.496	16.362	27.679	1.00	20.45	A
	ATOM	933	NH1	ARG	A	183		24.672	16.123	26.666	1.00	19.81	A
	ATOM	934	NH2	ARG	Α	183		25.224	17.338	28.539	1.00	17.11	A
	ATOM	935	C .	ARG	Α	183	•	29.206	15.577	23.302	1.00	20.02	A
	MOTA	936	0	ARG	Α	183		30.383	15.333	23.573	1.00	19.97	A
35	MOTA	937	N	PHE	Α	184	_	28.520	14.871	22.409	1.00	19.24	Α
	MOTA	938	CA	PHE	A	184	_	29.144	13.746	21.722	1.00	18.04	A
	MOTA	9.39	СВ	PHE	A	184		28.158	13.078	20.764	1.00	21.05	A
	MOTA	940	CG	PHE	A	184		28.719	11.857	20.098	1.00	22.67	A
	MOTA	941	CD1	PHE	Α	184		28.717	10.630	20.754		22.97	A
40	ATOM	942		PHE				29.317	11.949	18.850	1.00	19.97	A
	ATOM	943		PHE				29.308	9.510	20.176		23.53	A
	ATOM	944		PHE				29.915	10.833	18.263		24.11	A
	ATOM '	945	cz	PHE	А	184	-	29.910	9.613	18.928		22.97	A
	ATOM.	946	С	PHE	А	184		30.403	14.127	20.941	1.00	17.99	A
45	ATOM	947	0	PHE				31.461	13.531	21.130		18.89	A
	MOTA	948	N	TYR				30.292	15.110	20.056		15.73	A
	ATOM	949	CA	TYR				31.443	15.519	19.265		15.72	A
	ATOM	950	CB	TYR				30.992	16.413	18.111		17.33	A
	ATOM	951	CG	TYR			_	30.364	15.584	17.015		19.37	A
50	MOTA	952		TYR				31.159	14.809	16.168		16.53	A
	ATOM	953		TYR				30.590	13.952	15.232		18.12	A
	ATOM	954		TYR				28.976	15.484	16.892		18.18	A
	ATOM	955		TYR				28.398	14.623	15.956		18.90	A
	ATOM	956	CZ	TYR				29.211	13.861	15.133		18.41	A
55	ATOM	957	OH	TYR				28.650	12.995	14.218		20.48	A
	ATOM	958	С	TYR				32.544	16.172	20.083		15.79	A
	ATOM	959	0	TYR				33.720	16.015	19.766		17.69	A
	ATOM	960	N	THR				32.176	16.887	21.142		15.68	, A
	ATOM	961	CA	THR	Α	186		33.184	17.504	21.997	1.00	16.03	A

	ATOM	9.62	CB	THR.	Α	186		32.559	18.403	23.094	1.00	16.62	Α
	ATOM	963	OG1				•	31.866	19.503	22.481	1.00	14.79	· A
	ATOM	964	CG2					33.656	18.953	24.019	1.00		A
				THR				33.954	16.375	22.680	1.00		A
_	ATOM	965	С					35.176	16.443	22.823		13.77	A
5	MOTA	966	0	THR									
	MOTA	.967	N	ALA				33.234	15.333	23.097		14.06	A
	ATOM	968	CA	ALA				33.869	14.196	23.757		14.74	
	ATOM	969	CB	ALA	Α	187		32.810	13.195	24.224	1.00		A
	ATOM	970	C	ALA	Α	187		34.875	13.509			14.41	A
10	ATOM	971	0	ALA	Α	187		35.972	13.136	23.247	1.00		A
	ATOM	972	N	GLU	Α	188		34.516	13.340	21.549	1.00	14.01	A
	ATOM	973	CA	GLU				35.443	12.704	20.615	1.00	13.50	A
•	ATOM	974	CB	GLU				34.782	12.449	19.251	1.00	12.85	A
		975	CG	GLU				33.622	11.454	19.282	1.00	12.71	A
1.5	ATOM			GLU				33.464	10.685	17.979		15.01	A
15	ATOM	976	CD					33.687	11.275	16.899		13.21	A
	ATOM	977		GLU						18.031		17.69	A
	ATOM	978		GLU				33.110	9.484				A
	ATOM	979	С	GLU				36.682	13.582	20.436		13.34	
	ATOM	980	0	GLU				37.803	13.085	20.408		14.69	A
20	ATOM	981	N	ILE	Α	189		36.486	14.893	20.326		13.52	A
	ATOM	982	CA	ILE	A	189		37.627	15.787	20.159		13.35	. A
	ATOM	983	CB	ILE	Α	189		37.169	17.247	19.939		13.95	A
	ATOM	984		ILE				38.381	18.165	19.822	1.00	12.47	A
	ATOM	985		ILE				36.302	17.332	18.671	1.00	13.44	A
25	ATOM	986		ILE				35.588	18.664	18.491	1.00	14.29	A
23		987	C	ILE				38.530	15.702	21.394	1.00	14.63	A
	MOTA			ILE				39.753	15.595	21.271		12.97	A
	ATOM	988	0					37.927	15.751	22.582		14.35	Ä
	MOTA	989	N	VAL				38.684	15.655	23.832		13.22	A
	MOTA	990	CA	VAL						25.061		14.28	A
30	MOTA	991	CB	VAL				37.743	15.690	26.326		15.08	A
	MOTA	992		VAL				38.509	15.267			12.08	A
	ATOM	993	CG2	LAV				37.160	17.082	25.233			A
	MOTA	994	С	$_{ m LAV}$				39.468	14.338	23.859		14.61	A
	MOTA	995	0	VAL	Α	190		40.634	14.304	24.250		13.72	
35	ATOM .	996	N	SER	Α	191		38.825	13.254	23.432		15.26	A
	ATOM	997	CA	SER	A	191		39.478	11.943	23.421		16.81	A
	ATOM	998	CB	SER	A	191		38.470	10.857	23.041		16.14	A
	ATOM	999	OG	SER	A	191		39.018	9.569	23.238		16.94	A
	ATOM	1000	C			191		40.649	11.928	22.441	1.00	16.58	A
40	ATOM	1001	ō			191		41.697	11.335	22.713	1.00	13.96	A
70	ATOM	1002	N			192		40.468	12.586	21.300	1.00	15.26	A
	ATOM	1002	CA			192		41.518	12.645	20.292	1.00	14.37	A
		1003	CB			192		40.989	13.296	19.016	1.00	14.43	A
	MOTA							42.695	13.440	20.845		16.46	Α
	ATOM	1005	С			192				20.697		17.96	. A
45	ATOM	1006	0	ALA	A	192		43.851	13.038	21.496	1 00	15.02	A
	ATOM	1007	N			193		42.401	14.563	22.067	1.00	15.42	A
	ATOM	1008	CA			193		43.459	15.392				_
	ATOM	1009	CB			193		42.884	16.712	22.600			
	ATOM	1010	CG			193		42.445	17.721	21.525		15.97	A
. 50	ATOM .	1011		LEU				41.869	18.979	22.190		13.97	A
	ATOM	1012	CD2	LEU	Α	193		43.642	18.088	20.655		14.58	A
	ATOM	1013	С	LEU	Α	193		44.211	14.659	23.174		14.49	A
	ATOM	1014	0			193		45.427	14.813	23.310		16.56	· A
	ATOM	1015	N			194		43.500	13.870	23.975	1.00	13.96	A
55	ATOM	1016	CA			194		44.179	13.123	25.032	1.00	14.08	A
55	ATOM	1017	CB			194		43.190	12.295	25.857		14.65	A
		1017	CG			194		43.882	11.301	26.789		17.09	A
	ATOM					194		42.924	10.592	27.730		19.59	A
	ATOM	1019	CD OF 1	L GLU				41.809	10.332	27.295		19.25	А
	ATOM	1020	OE.	r GTiO	A	174		41.009	10.231	2			

	MOTA	1021	OE2	GLU	Α	194	43.302	10.380	28.906	1.00	20.20	A
	ATOM	1022	C	GLU	Α	194	45.208	12.199	24.386	1.00	13.57	A
	MOTA	1023	0	GLU	A	194	46.337	12.093	24.847		14.23	A
	MOTA	1024	N	TYR	Α	195·	44.822	11.544	23.301	1.00	14.89	A
5	ATOM	1025	CA	TYR	Α	195	45.743	10.642	22.618	1.00	16.58	A
	ATOM	1026	CB	TYR			45.030	9.910	21.488	1.00	17.29	A
	ATOM	1027	CG	TYR			45.956	9.058	20.649	1.00	17.92	A
	ATOM	1028		TYR			46.347	7.788	21.077	1.00	17.96	A
	ATOM	1029		TYR			47.203	6.996	20.304	1.00		A
10	ATOM	1030	CD2				46.445	9.524	19.428	1.00		A
10	ATOM	1031		TYR			47.299	8.744	18.650	1.00		A
		1031	CZ	TYR			47.671	7.481	19.094	1.00		A
	ATOM	1032		TYR			48.506	6.705	18.325	1.00		A
	ATOM		ОН				46.917	11.419	22.035	1.00		A
1.5	ATOM	1034	С	TYR								
15	ATOM	1035	0	TYR			48.081	11.047	22.203	1.00		A
	ATOM	1036	N	LEU			46.599	12.507	21.347	1.00		A
	MOTA	1037	CA	LEU			47.619	13.328	20.720	1.00		A
	MOTA	1038	CB	LEU			46.969	14.502	19.982	1.00		A
	MOTA	1039	CG	LEU			47.834	15.203	18.935	1.00		A
20	ATOM	1040		LEU			48.222	14.206	17.841	1.00		A _.
	MOTA	1041	CD2	LEU	A	196	47.060	16.375	18.338	1.00		A
	ATOM	1042	C	LEU	A	196	48.592	13.844	21.763	1.00	17.75	A
	MOTA	1043	0	LEU	Α	196	49.801	13.644	21.649	1.00		A
	MOTA	1044	N	HIS	Α	197	48.064	14.495	22.792	1.00	17.12	A
25	MOTA	1045	CA	HIS	Α	197	48.913	15.042	23.842	1.00	18.47	A
	ATOM	1046	CB	HIS	Α	197	48.069	15.866	24.817	1.00	15.90	A
	ATOM	1047	CG	HIS	Α	197	47.571	17.152	24.231	1.00	19.15	A
	ATOM	1048	CD2	HIS	A	197	47.830	17.745	23.038	1.00	18.22	A
	ATOM	1049	ND1	HIS	Α	197	46.704	17.992	24.897	1.00	17.47	A
30	ATOM	1050		HIS			46.450	19.047	24.139	1.00	19.74	A
-	ATOM	1051		HIS			47.119	18.921	23.007	1.00	15.69	A
	ATOM	1052	C	HIS			49.696	13.958	24.572	1.00	19.40	Α
	ATOM	1053	ō	HIS			50.823	14.192	25.021	1.00		A
	ATOM	1054	N	GLY			49.106	12.770	24.679	1.00		A
35	ATOM	1055	CA	GLY			49.793	11.675	25.339	1.00		A
55	ATOM	1056	C	GLY			51.075	11.307	24.612	1.00		A
	ATOM	1057	ō	GLY			51.963	10.682	25.186	1.00		A
	ATOM	1057	N	LYS			51.174	11.687	23.341	1.00		A
	ATOM	1059	CA	LYS			52.368	11.401	22.549	1.00		A
40		1060		LYS			51.990	10.905	21.154	1.00		A
40	MOTA		CB	LYS			51.378	9.520	21.133	1.00		A.
	ATOM	1061	CG				51.370	9.002	19.708	1.00		A
	ATOM	1062	CD	LYS			50.832	7.559	19.682	1.00		A
	MOTA	1063	CE	LYS .			51.646	6.691	20.581	1.00		A
4.50	MOTA	1064	NZ									A
45	ATOM	1065	C	LYS					22.414			
	MOTA	1066	0	LYS			54.144	12.669	21.568	1.00		A
	ATOM	1067	N	GLY			52.997	13.638	23.243	1.00		A
	MOTA	1068	CA	GLY			53.790	14.853	23.203	1.00		A
	ATOM	1069	С			200 `	53.665	15.632	21.907	1.00		Α.
50	ATOM	1070	0	GLY .			54.632	16.231	21.439	1.00		A
	ATOM	1071	N	ILE .			52.475	15.630	21.320	1.00		A
	MOTA	1072	CA	ILE .			52,252	16.355	20.080	1.00		A
	ATOM	1073	CB	ILE .			51.784	15.414	18.955	1.00		A
	ATOM	1074		ILE .			51.414	16.226	17.716	1.00		A
55	ATOM	1075	CG1	ILE .	Α	201	52.880	14.395	18.636	1.00		A
	ATOM	1076	CD1	ILE .	Α	201	52.408	13.258	17.745	1.00		A
	ATOM	1077	С	ILE .	Α	201	51.193	17.425	20.270	1.00		A
•	ATOM	1078	0	ILE .			50.121	17.161	20.817	1.00		A
	MOTA	1079	N	ILE .			51.508	18.633	19.815	1.00	19.94	A

	ATOM	1080	CA	ILE	Α	202	50.60	1	19.772	19.891	1.00 20.45	· A
	ATOM	1081	СВ	ILE	Α	202	51.35		21.040	20.356	1.00 22.21	
	ATOM	1082	CG2	2 ILE	A	202	50.38		22.220	20.470	1.00 22.67	
	ATOM	1083		LILE			52.03		20.775	21.700	1.00 24.19	
5	ATOM	1084		LILE			52.91		21.920	22.169	1.00 25.39	
Ŭ	ATOM	1085	C			202	50.10		19.999	18.464	1.00 20.71	
	ATOM	1086	ō			202	50.910		20.067			
	ATOM	1087	N	HIS						17.538	1.00 19.48	
							48.795		20.108	18.270	1.00 18.65	
10	ATOM	1088	CA	HIS			48.280		20.319	16.919	1.00 18.02	
10	ATOM	1089	CB	HIS			46.775		20.057	16.874	1.00 16.31	
	ATOM	1090	CG	HIS			46.199		20.136	15.495	1.00 18.36	
	ATOM	1091		HIS			46.043		21.186	14.655	1.00 16.42	
	MOTA	1092		. HIS			45.759		19.026	14.806	1.00 19.50	A
	ATOM	1093		. HIS			45.359	9	19.389	13.600	1.00 17.64	A
15	MOTA	1094		HIS	Α	203	45.522	2	20.694	13.483	1.00 20.87	. A
	ATOM	1095	С	HIS	A	203	48.589	9	21.738	16.405	1.00 18.92	. A
	ATOM	1096	0	HIS	Α	203	49.073	3	21.906	15.282	1.00 16.21	
	MOTA	1097	N	ARG	Α	204	48.301	1	22.744	17.232	1.00 18.60	
	MOTA	1098	CA	ARG	Α	204	48.552	2	24.157	16.914	1.00 19.81	
20	MOTA	1099	CB	ARG			49.998		24.365	16.458	1.00 21.61	
	MOTA	1100	CG	ARG	Α	204	51,024		24.137	17.550	1.00 23.82	
	MOTA	1101	CD	ARG			52.323		24.870	17.252	1.00 27.62	
	ATOM	1102		ARG			52.932		24.449	15.994	1.00 27.02	
	ATOM	1103	CZ	ARG			54.125		24.861	15.572	1.00 23.43	
25	ATOM	1104		ARG			54.835		25.706	16:311	1.00 33.10	
23	ATOM	1105		ARG			54.614					
	ATOM	1105	C	ARG					24.426	14.418	1.00 30.25	
	MOTA	1107		ARG			47.624		24.830	15.905	1.00 20.03	
			0				47.711		26.038	15.698	1.00 20.88	
20	MOTA	1108	N	ASP			46.755		24.071	15.255	1.00 18.96	
30	MOTA	1109	CA	ASP			45.828		24.692	14.325	1.00 17.90	
	ATOM	1110	CB	ASP			46.418		24.741	12.914	1.00 18.95	
	MOTA	1111	CG	ASP			45.655		25.688	12.008	1.00 20.36	
	ATOM	1112		ASP .			44.939		26.560	12.545	1.00 20.35	
	MOTA	1113		ASP .			45.772		25.573	10.771	1.00 22.49	A
35	ATOM	1114	С	ASP .			44.500)	23.956	14.328	1.00 19.60	A
	ATOM	1115	0	ASP .			43.876	5	23.751	13.287	1.00 21.53	A
	MOTA	1116	N	LEU .	Α	206	44.063	3	23.569	15.521	1.00 18.53	A
	MOTA	1117	CA	LEU .	A	206	42.813	3	22.851	15.667	1.00 19.18	A
	ATOM	1118	CB	LEU .	Α	206	42.693	3	22.295	17.087	1.00 18.94	А
40	MOTA	1119	CG	TEA Y	Α	206	41.511	L	21.358	17.346	1.00 23.10	A
	ATOM	1120	CD1	LEU 2	Α	206	41.615	5	20.142	16.436	1.00 23.01	A
	MOTA	1121	CD2	LEU 2	A	206	41.504		20.933	18.808	1.00 22.97	A
	ATOM	1122	C -	LEU Z	A	206	41.639)	23.772	15.361	1.00 19.05	· A
	ATOM	1123	0	LEU I	A	206	41.556		24.880	15.886	1.00 19.25	A
45	ATOM	1124	N	LYS 2			40.740		23.307	14.500	1.00 17.54	A
	ATOM	1125	CA	LYS 2			39.564		24.081	14.110	1.00 18.60	A
	ATOM	1126	СВ	LYS			39.980		25.248	13.196	1.00 18.98	A
	ATOM	1127	CG	LYS A			40.786		24.817	11.982	1.00 18.20	
	ATOM	1128	CD	LYS A			41.246		26.000			A
5 0	ATOM	1129	CE	LYS A						11.139	1.00 21.42	A
50	ATOM	1130	NZ	LYS A			42.223		25.537	10.062	1.00 23.21	A
							42.561		26.604	9.084	1.00 29.61	A
	ATOM	1131	C	LYS A			38.566		23.181	13.388	1.00 18.18	A
	ATOM	1132	0	LYS A			38.921		22.100	12.915	1.00 18.11	A
<i>E E</i>	ATOM	1133	N	PRO A			37.298		23.614	13.293	1.00 20.26	Α
55	ATOM	1134	CD	PRO A			36.713		24.833	13.882	1.00 18.79	A
	MOTA	1135	CA	PRO A			36.272		22.814	12.616	1.00 19.67	A
	ATOM	1136	CB	PRO A			35.063		23.742	12.608	1.00 19.45	Α
	ATOM	1137	CG	PRO A			35.231		24.509	13.891	1.00 21.81	A
	ATOM	1138	С	PRO A	1	208	36.674		22.372	11.209	1.00 21.04	A

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	MOTA	1139	0	PRO 2	Ą	208		36.264	21.307	10.751	1.00 21.19	A
	ATOM	1140	N	GLU 2	A	209		37.474	23.188	10.528	1.00 21.69	Α
	ATOM	1141	CA	GLU 2	A	209		37.928	22.872	9.170	1.00 22.64	A
	ATOM	1142	СВ	GLU				38.644	24.084	8.558	1.00 23.65	A
5	ATOM	1143	CG	GLU 2	A	209		39.253	23.825	7.185	1.00 27.24	A
,	ATOM	1144	CD	GLU Z				40.155	24.958	6.716	1.00 29.40	A
		1145		GLU				39.660	26.094	6.553	1.00 29.68	A
•	ATOM			GLU A				41.363	24.711	6.511	1.00 30.07	A
	ATOM	1146								9.159	1.00 22.28	A
	MOTA	1147	C	GLU I				38.879	21.668	8.170	1.00 22.20	A
10	ATOM	1148	0	GLU				38.955	20.933			
	MOTA	1149	N	ASN .				39.600	21.490	10.263	1.00 19.90	A
	MOTA	1150	CA	ASN .				40.574	20.412	10.436	1.00 19.44	A
	ATOM	1151	CB	ASN .	A	210		41.744	20.912	11.287	1.00 20.07	A
	ATOM	1152	CG	ASN .	A	210		42.746	21.698	10.479	1.00 25.77	A
15	ATOM	1153	OD1	ASN .	A	210		43.571	22.427	11.029	1.00 26.73	A
	ATOM	1154	ND2	ASN 3	A	210		42.687	21.548	9.158	1.00 25.15	Α
	ATOM	1155	С	ASN .	A	210		40.005	19.151	11.078	1.00 18.63	A
	ATOM	1156	Ō	ASN .				40.712	18.154	11.234	1.00 18.29	A
	ATOM	1157	N	ILE				38.739	19.202	11.469	1.00 16.31	A
20	ATOM	1158	CA	ILE .				38.090	18.058	12.085	1.00 15.49	A
20	ATOM	1159	CB	ILE .				37.336	18.488	13.354	1.00 15.40	A
	ATOM	1160		ILE .				36.582	17.311	13.950	1.00 14.59	A
		1161		ILE .				38.342	19.046	14.365	1.00 15.91	A
	ATOM							37.720	19.669	15.590	1.00 15.98	A
~~	MOTA	1162		ILE .			,			11.059	1.00 13.30	. A
25	ATOM	1163	C	ILE .				37.131	17.485		1.00 17.20	A
	ATOM	1164	0	ILE .				35.995	17.947	10.926	1.00 15.10	A
	MOTA	1165	N	LEU				37.599	16.486	10.317		
	ATOM	1166	CA	LEU				36.784	15.875	9.274	1.00 17.08	A
	MOTA	1167	CB	LEU				37.685	15.249	8.202	1.00 17.78	
30	MOTA	1168	CG	LEU				38.785	16.157	7.640	1.00 18.92	A
	ATOM	1169		LEU				39.476	15.450	6.485	1.00 22.09	A
	ATOM	1170	CD2	LEU	A	212		38.188	17.482	7.166	1.00 19.91	A
	ATOM	1171	С	LEU	A	212		35.843	14.825	9.837	1.00 18.35	A
	ATOM	1172	0	LEU	A	212		35.957	14.433	11.002	1.00 19.39	A.
35	ATOM	1173	N	LEU	A	213		34.915	14.368	9.000	1.00 17.84	A
	ATOM	1174	CA	LEU	Α	213		33.942	13.362	9.403	1.00 19.94	A
	ATOM	1175	CB	LEU				32.556	14.004	9.487	1.00 20.84	A
	ATOM	1176	CG	LEU				32.396	15.059	10.583	1.00 20.31	A
	ATOM	1177		LEU				31.124	15.837	10.367	1.00 22.75	A
40	ATOM	1178		LEU				32.379	14.378	11.940	1.00 23.93	Α
40	ATOM	1179	C			213		33.914	12.187	8.426	1.00 20.98	A
	ATOM	1180	Ö	LEU				33.743	12.379	7.218	1.00 19.55	A
				ASN				34.088	10.970	8.935	1.00 20.44	A
	ATOM	1181	N	ASN				34.055	9.814	8.049	1.00 23.77	A
	ATOM	1182	CA							8.674	1.00 25.30	A
45	ATOM	1183	CB	ASN				34.745	8.596	9.948	1.00 23.30	A
	ATOM	1184	CG.	ASN				34.077	8.127			A
	MOTA	1185		ASN				32.908	8.422	10.206	1.00 34.43	
	ATOM	1186	ND2	ASN				34.818	7.369	10.752	1.00 33.85	· A
	ATOM	1187	С	ASN			•	32.618	9.466	. 7.693	1.00 24.07	A
50	ATOM	1188	0	ASN				31.672	10.113	8.150	1.00 19.94	A
	ATOM	1189	N	GLU	Α	215		32.459	8.433	6.879	1.00 25.77	A
	ATOM	1190	CA	GLU				31.138	8.003	6.445		A
	ATOM	1191	CB	GLU	A	215		31.275	6.796		1.00 31.98	A
	ATOM	1192	CG	GLU				29.970	6.334	4.896	1.00 40.22	. A
55	ATOM	1193	CD	GLU				30.182	5.312	3.795	1.00 44.27	A
	ATOM	1194		GLU				30.817	4.268	4.065	1.00 46.46	A
	ATOM	1195		GLU				29.716	5.556	2.660	1.00 46.13	A.
	ATOM	1196	C	GLU				30.188	7.673	7.601	1.00 28.41	A
	ATOM	1197	Ö	GLU				28.971	7.769	7.447	1.00 28.52	A
	AION	2271	~	0.110	4.1	213		22.274				

	ATOM	1198	N	ASP	Α	216	-	30.73	37	7.287	8.752	1.00	26.77	Α
	ATOM	1199	CA			216		29.93	14	6.953	9.917		27.28	A
	ATOM	1200	CB			216		30.53		5.795	10.696		31.27	A
	ATOM	1201	CG			216		30.39		4.466	9.979		37.61	A
5	ATOM	1202		ASP				29.27			9.499		39.45	A
•	ATOM	1203		ASP				31.38		3.710			41.84	
	ATOM	1203	C			216		29.69		8.135	10.862		26.37	A
	ATOM	1205	0			216		29.13		7.984				A
	ATOM	1205				217		30.15			11.950		25.73	A
10			N			217				9.306	10.441		23.02	A
10	ATOM	1207	CA					30.01		10.527	11.218		21.83	A
	ATOM	1208	CB	MET				28.53		10.789	11.517		23.24	A
	ATOM	1209	CG	MET				27.74		11.186	10.274		22.98	A
	MOTA	1210	SD	MET				28.46		12.616	9.430		.27.57	Α
1.5	ATOM	1211	CE	MET				27.67		13.974	10.332		26.68	A
15	ATOM	1212	C	MET				30.84		10.618	12.502		21.51	A
	ATOM	1213	0	MET				30.47		11.323	13.440		18.62	A
	ATOM	1214	N	HIS				31.95		9.892	12.544	1.00	20.10	A
	ATOM	1215	CA	HIS				32.87		9.964	13.678		19.86	A
	ATOM	1216	CB	HIS				33.48		8.594	13.977		20.21	A
20	ATOM	1217	CG	HIS				32.55		7.667	14.698	1.00	22.40	A
	ATOM	1218		HIS				31.91		6.547	14.287		21.27	A
	MOTA	1219		HIS				32.17		7.863	16.011	1.00	19.59	A
	ATOM	1220		HIS				31.34		6.902	16.379		21.88	A
	ATOM	1221	NE2	HIS				31.16		6.091	15.351		22.08	A
25	ATOM	1222	С	HIS	Α	218		33.94		10.921	13.172	1.00	19.10	A
	ATOM	1223	0	HIS	A	218		34.17	70	11.004	11.965	1.00	20.31	Α
	ATOM	1224	N	I·LE				34.61	.7	11.638	14.067	1.00	17.21	A
	ATOM	1225	CA	ILE	Α	219		35.62	8	12,586	13.618	1.00	15.26	A
	ATOM	1226	CB	ILE	Α	219		35.98	37	13.614	14.716	1.00	15.38	A
30	ATOM	1227		ILE				34.72		14.305	15.221	1.00	14.58	A
	MOTA	1228		ILE				36.73		12.919	15.864		14.46	A
	ATOM	1229	CD1	ILE				37.27		13.885	16.911		13.74	A
	ATOM	1230	C	ILE				36.92		11.944	13.161		16.21	A
	ATOM	1231	0	ILE	Α	219		37.23		10.799	13.500	1.00	15.88	A
35	ATOM	1232	N	GLN	Α	220		37.67	7	12.711	12.378	1.00	15.62	A
•	ATOM	1233	CA	GLN	Α	220		38.98	0	12.316	11.876	1.00	17.84	Α
	ATOM	1234	CB	GLN	Α	220.		38.87	2	11.595	10.525	1.00	20.00	A
	MOTA	1235	CG	GLN	Α	220		38.46	3	10.129	10.659	1.00	26.97	A
	ATOM	1236	CD	GLN	Α	220		38.64	8	9.343	9.372	1.00	29.95	\mathbf{A}'
40	MOTA	1237	OEl	GLN	Α	220		37.96	8	9.590	8.373	1.00	33.12	A
	MOTA	1238	NE2	GLN	A	220		39.57	8	8.393	9.389	1.00	30.47	Α
	MOTA	1239	C	GLN	Α	220		39.75	7	13.610	11.735	1.00	17.00	A
	MOTA	1240	0	GLN	Α	220		39.60	9	14.339	10.751	1.00	18.27	A
	ATOM	1241	N	ILE				40.56		13.906	12.746		14.34	A
45	ATOM	1242	CA	ILE	Α	221		41.36	1	15.120	12.753	1.00	14.46	A
	ATOM	1243	CB	ILE				41.86	7	15.416	14.175	1.00	12.30	A
	ATOM	1244	CG2	ILE	Α	221		42.76	4	16.656	14.167	1.00	14.78	A
	ATOM ·	1245	CG1	ILE	Α	221		40.66	0	15.613	15.102	1.00	13.92	A
	ATOM	1246	CD1	ILE	Α	221		41.00	3	15.901	16.543	1.00	15.06	A
50	ATOM	1247	С	ILE	Α	221		42.53	6	14.996	11.783	1.00	15.44	A
	ATOM	1248	0	ILE	Α	221		43.10	6	13.915	11.613	1.00	13.93	A
	MOTA	1249	N	THR	Α	222		42.87	7	16.101	11.127	1.00	15.36	A
	ATOM	1250	CA	THR				43.98	0	16.098	10.174	1.00	17.52	A
	ATOM	1251	CB	THR				43.47	0	15.836	8.750	1.00	19.92	A
55	ATOM	1252	OG1	THR	Α	222		44.58	7	15.637	7.875		18.78	Α
	ATOM	1253	CG2	THR	A	222		42.63	0	17.018	8.257	1.00	18.16	A
	MOTA	1254	С	THR				44.73		17.428	10.192		19.60	Α
	ATOM	1255	0	THR				44.50	9	18.257	11.084		18.59	A
	ATOM	1256	N	ASP	Α	223		45.63	0	17.610	9.216	1.00	18.69	A

	. ATOM	1257	CA	ASP.	A 22	3 46.440	18.825	9.069	1.00	20.12	А
	ATOM	1258	CB	ASP :	A 22	3 45.532	20.065	9.108	1.00	23.51	A
	ATOM	1259	CG	ASP I			21.335	8.670		27.09	A
	ATOM	1260	OD1	ASP .			21.227	7.975		26.28	A
5	ATOM	1261		ASP 2			22.438	9.009		26.15	
,	ATOM	1262		ASP A			18.913	10.150			A
		1263		ASP I			19.751			21.73	A
	ATOM		0					11.055		22.76	. A
	ATOM	1264	N	PHE			18.063	10.027		20.75	A
	ATOM	1265	CA	PHE I			17.988	11.009		20.11	A
10	ATOM	1266	CB	PHE 2			16.527	11.424		20.62	A
	MOTA	1267	CG	PHE A	A 22	48.682	15.991	12.263	1.00	21.41	A
	MOTA	1268	CD1	PHE Z	A 22	4 48.598	16.312	13.614	1.00	23.05	A
	MOTA	1269	CD2	PHE A	A 22	4 47.681	15.212	11.693	1.00	22.27	A
	ATOM	1270	CE1	PHE 2	A 22	4 47.528	15.868	14.389	1.00	23.30	A
15	ATOM	1271	CE2	PHE Z	A 22	4 46.606	14.763	12.457	1.00	21.11	A
-	ATOM	1272	CZ	PHE Z			15.093	13.807		22.02	. A
	ATOM	1273	c	PHE A			18.583	10.619		20.45	A
	MOTA	1274	ŏ	PHE A			18.547	11.407		20.73	A
	ATOM	1275	N	GLY A			19.125	9.412		22.02	A
20							19.713				
20	ATOM	1276	CA	GLY A				8.981		22.66	A
	ATOM	1277	С	GLY A			20.822	9.920		24.99	A
	MOTA	1278	0	GLY A			21.041	10.122		24.52	
	ATOM	1279	N	THR A			21.524	.10.508		23.50	A
	MOTA	1280	CA	THR A			22.613	11.416		25.16	A
25	ATOM	1281	CB	THR A	A 22	6 51.199	23.829	11.160	1.00	24.76	A
	ATOM	1282	OG1	THR A	A 2,2	6 . 49.831	23.410	11.113	1.00	22.68	A
	ATOM	1283	CG2	THR A	A 22	6 51.571	24.490	9.834	1.00	25.00	Α
	MOTA	1284	С	THR A	A 22	6 52.046	22.233	12.894	1.00	25.79	A
	ATOM	1285	0	THR A	A 22	6 52.019	23.100	13.768	1.00	24.54	A
30	ATOM	1286	N	ALA A			20.935	13.173	1.00	24.97	A
	ATOM	1287	CA	ALA A			20.475	14.550		25.49	A
	ATOM	1288	CB	ALA A			18.993	14.607		22.85	A
	MOTA	1289	C	ALA A			20.715	15.149		27.70	. A
	ATOM	1290	0	ALA A			21.047	14.435		26.60	A
25							20.558			28.53	A
35	ATOM	1291	N	LYS A				16.461			
	MOTA	1292	CA	LYS A			20.745	17.149		32.12	A
	MOTA	1293	CB	LYS A			21.974	18.054		33.81	A
	ATOM	1294	CG	LYS A			22.294	18.765		41.23	A
	ATOM	1295	CD	LYS A			22.725	17.768		47.57	A
40	MOTA	1296	CE	LYS A	1 22	8 58.401	23.056	18.462		49.82	A
	MOTA	1297	NZ	LYS A	1 22	8 59.459	23.425	17.480	1.00	51.49	· А
	ATOM	1298	С	LYS A	A 22	8 55.019	19.504	17.985	1.00	33.25	A
	ATOM	1299	· 0	LYS A	A 22	8 54.190	19.129	18.815	1.00	33.70	A
	ATOM	1300	N	VAL A			18.860	17.756	1.00	33.64	A
45	MOTA	1301	CA	VAL A	22	9 56.516	17.661	18.501	1.00	34.66	A
	ATOM	1302	CB	VAL A			16.646	17.609		33.50	A
	ATOM	1303		VAL A			15.419	18.415		32.34	A
	ATOM	1304		VAL A			16.264	16.436		34.25	A
		1305	C				18.035	19.668		37:57	A
50	ATOM			VAL A							
50	ATOM	1306	0	VAL A			18.392	19.474		35.91	A
	ATOM	1307	N	LEU A			17.948	20.878		40.57	A
	ATOM	1308	CA	LEU A			18.289	22.088		46.10	A
	MOTA	1309	CB	LEU A			18.417	23.270		44.71	. A
	ATOM	1310	CG	LEU A			19.545	23.207		44.50	· A
55	ATOM	1311		LEU A			19.430	24.383		44.39	A
	ATOM	1312	CD2	LEU A			20.885	23.214		44.81	A
	ATOM	1313	С	LEU A	23	0 58.695	17.279	22.440	1.00	50.42	Α
	ATOM	1314	0	LEU A			16.104	22.089	1.00	51.64	A
	ATOM	1315	N	SER A			17.756	23.145	1.00	55.81	A

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	MOTA	1316	CA	SER A	231		60.824	16.914	23.583	1.00 61.14	A
	ATOM	1317	CB .	SER A	231	-	62.077	17.200	22.750	1.00 61.27	A
	ATOM	1318	OG	SER A	231		62.444	18.568	22.823	1.00 62.85	A
	ATOM	1319	С	SER A	231		61.124	,17.126	25.071	1.00 64.65	A
5	ATOM	1320	0	SER F	231		61.392	16.164	25.794	1.00 65.70	A
	ATOM	1321	N	PRO P			61.081	18.387	25.549	1.00 67.54	A
	MOTA	1322	CD	PRO P			60.854	19.651	24.823	1.00 68.60	A
	ATOM	1323	CA	PRO F			61.358	18.655	26.966	1.00 68.74	A
	ATOM	1324	СВ	PRO P			61.109	20.158	27.086	1.00 68.83	A
10	ATOM	1325	CG	PRO P			61.505	20.666	25.737	1.00 68.96	A
	ATOM	1326	C	PRO P			60.460	17.846	27.899	1.00 69.17	A
•	ATOM	1327	ō	PRO P			59.335	17.494	27.541	1.00 69.94	A
	ATOM	1328	N	ALA A			57.424	23.198	27.637	1.00 80.06	A
	ATOM	1329	CA	ALA A			56.783	23.047	26.335	1.00 79.29	A
15	ATOM	1330	CB	ALA A			55.275	22.907	26.512	1.00 78.64	A
13	ATOM	1331	C,	ALA A	•		57.092	24.239	25.433	1.00 79.07	A
	ATOM	1332	Ö	ALA A			56.250	25.113	25.249	1.00 79.47	A
	ATOM	1333	N	ALA A			58.297	24.280	24.871	1.00 73.47	A
	ATOM	1334	CA	ALA A			58.683	25.383	23.992	1.00 78.50	A
20	ATOM	1335	CB	ALA A			60.186	25.347	23.728	1.00 78.50	A
20		1336	CD	ALA A			57.920	25.327	22.673	1.00 78.30	A
	ATOM ATOM	1337	0	ALA A			57.243	24.341	22.375	1.00 78.15	A
	ATOM	1338	N	ALA A			58.027	26.393	21.887	1.00 77.28	Ā
		1339	CA	ALA A			57.338		20.603	1.00 77.28	A
25	ATOM	1340	CB	ALA A			55.849	26.452 26.489	20.827	1.00 76.27	A.
23	ATOM ATOM	1340	СВ	ALA A			57.766	27.667	19.793	1.00 75.38	A
	ATOM	1341	0	ALA A			58.955	27.955	19.700	1.00 75.89	A
	ATOM	1342	N	ASN A			56.781	28.357	19.700	1.00 73.89	A
	ATOM	1344	CA	ASN A			56.967	29.553	18.389	1.00 73.93	A
30	ATOM	1344	CB	ASN A			58.151	30.400	18.874	1.00 71.07	A
30	ATOM	1345	CG	ASN A			59.459	30.400	18.174	1.00 71.47	A
	ATOM	1347		ASN A			59.575	30.149	16.174	1.00 72.00	A
	ATOM	1347		ASN A			60.470	29.665	18.964	1.00 72.03	A
	ATOM	1349	C	ASN A			57.188	29.178	16.928	1.00 71.91	A
35	ATOM	1350	o	ASN A			57.480	28.024	16.624	1.00 05.41	Ā
55	ATOM	1351	N	ALA A			57.055	30.165	16.038	1.00 66.62	A
	ATOM	1352	CA	ALA A			57.246	30.103	14.585	1.00 63.94	A
	ATOM	1353	C	ALA A			55.952	30.080	13.772	1.00 60.63	A
	ATOM	1354	Ö	ALA A			55.840	30.880	12.845	1.00 61.29	A
40	ATOM	1355	СВ	ALA A			57.979	28.704	14.246	1.00 65.23	A
	ATOM	1356	N	PHE A			54.984	29.236	14.113	1.00 56.72	A
	ATOM	1357	CA	PHE A			53.712	29.196	13.394	1.00 52.53	A
	ATOM	1358	СВ	PHE A			53.419	27.767	12.923	1.00 49.14	A
	ATOM	1359	CG	PHE A			52.040	27.590	12.354	1.00 47.38	A
45	ATOM	1360		PHE A			51.731	28.067	11.085	1.00 47.69	A
	ATOM	1361		PHE A			51.038	26.975	13.102	1.00 45.45	A
	ATOM	1362		PHE A			50:445	27.937	10.565	1.00 46.75	A
	ATOM	1363		PHE A			49.751	26.840	12.594	1.00 45.41	A
	ATOM	1364	CZ	PHE A		٠.	49.453	27.323	11.322	1.00 46.55	A
50	ATOM	1365	C	PHE A			52.534	29.688	14.229	1.00 50.08	A
	ATOM	1366	o	PHE A			52.502	29.505	15.444	1.00 49.86	A
	ATOM	1367	N	VAL A			51.566	30.305	13.557	1.00 47.67	A
	ATOM	1368	CA	VAL A			50.355	30.809	14.200	1.00 46.21	A
	MOTA	1369	СВ	VAL A			50.340	32.352	14.258	1.00 47.36	
55	ATOM	1370		VAL A			49.012	32.844	14.825	1.00 47.54	Α .
	ATOM	1371		VAL A			51.497	32.842	15.109	1.00 48.50	A
	ATOM	1372	С	VAL A			49.150	30.342	13.389	1.00 44.12	· A
	ATOM	1373	Ō	VAL A			48.956	30.765	12.247	1.00 44.46	A
	ATOM	1374	N	GLY A			48.348	29.467	13.985	1.00 40.48	· A

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	MOTA	1375	CA	GLY A	244	47.176	28.941	13.306	1.00 37.65	A
•	ATOM	1376	С	GLY A	244	46.101	29.960	12.964	1:00 35.39	A
	MOTA	1377	0	GLY A	244	46.313	31.168	13.065	1.00 35.92	A
	ATOM	1378	N	THR A	245	44.936	29.463	12.560	1.00 33.30	A
5	MOTA	1379	CA	THR A	245	43.813	30.312	12.184	1.00 30.20	A
-	ATOM	1380	CB	THR A	245	42.593	29.450	11.829	1.00 32.00	A
	ATOM	1381	OG1	THR A	245	42.952	28.573	10.755	1.00 32.81	A
	ATOM	1382	CG2	THR A	245	41.419	30.319	11.390	1.00 28.34	A
	ATOM	1383	С	THR A			31.296	13.296	1.00 27.96	A
10	ATOM	1384	0	THR A			30.907	14.434	1.00 25.46	A
	ATOM	1385	Ń	ALA A			32.576	12.938	1.00 25.22	A
	ATOM	1386	CA	ALA A			33.675	13.867	1.00 23.27	A
	ATOM	1387	CB	ALA A			34.955	13.082	1.00 22.94	A
	ATOM	1388	C	ALA A			33.475	14.934	1.00 21.27	A
15	ATOM	1389	ō	ALA A			33.705	16.114	1.00 20.93	A
13	ATOM	1390·	N	GLN A			33.047	14.536	1.00 19.67	A
	ATOM	1391	CA	GLN A			32.886	15.504	1.00 20.17	A
	ATOM	1392	CB	GLN A		38.608	32.535	14.779	1.00 21.89	· A
	ATOM	1393	CG	GLN A			33.076	13.355	1.00 26.18	A
20	ATOM	1394	CD	GLN A			33.794	13.064	1.00 27.30	A
20	ATOM	1395	OE1	GLN A			33.447	13.605	1.00 30.13	
	ATOM	1396		GLN A			34.792	12.189	1.00 28.70	
	ATOM	1397	C	GLN A			31.1849	16.595	1.00 19.43	A
	ATOM	1398	Ö	GLN A		39.546	31.883	17.648	1.00 18.93	A
25	ATOM	1399	N	TYR A			30.948	16.359	1.00 18.60	A
23	ATOM	1400	CA.	TYR A			29.896	17.329	1.00 19.20	A
	ATOM '	1401	CB		248	41.333	28.529	16.642	1.00 17.53	A
	ATOM	1402	CG	TYR A			28.362	15.927	1.00 19.32	A
	ATOM	1403		TYR A		38.859	28.010	16.625	1.00 17.69	A
30	ATOM	1404		TYR A			27.976	15.990	1.00 18.18	· A
50	ATOM	1405		TYR A			28.664	14.569	1.00 16.87	A
	ATOM	1406		TYR A			28.635	13.924	1.00 19.17	A
	ATOM	1407	CZ		248		28.295	14.643	1.00 19.46	Α
	ATOM	1408	ОН	TYR A			28.311	14.023	1.00 18.98	A
35	ATOM	1409	C	TYR A			30.039	17.993	1.00 20.42	A
55	ATOM	1410	ō		248		29.191	18.792	1.00 19.19	A
	ATOM	1411	N	VAL A		,	31.114	17.673	1.00 20.20	A
	ATOM	1412	CA	VAL A			31.343	18.251	1.00 20.91	A
	MOTA	1413	СВ	VAL A			32.532	17.570	1.00 21.18	A
40	ATOM	1414		VAL A			32.896	18.317	1.00 22.45	A
	ATOM	1415		VAL A			32.170	16.139	1.00 24.01	A
	ATOM	1416	С	VAL A	249	44.764	31.606	19.750	1.00 21.52	A
	ATOM	1417	0	VAL A			32.368	20.216	1.00 22.72	A
	ATOM	1418	N	SER A	250	45.654	30.965	20.503	1.00 20.70	Α
45	ATOM	1419	CA		A 250	45.697	31.133	21.951	1.00 21.65	A
	ATOM	1420	СВ	SER A		46.370	29.919	22.613	1.00 22.02	A
	MOTA	1421	OG	SER A			29.725	22.132	1.00 22.12	A
	ATOM	1422	С		250		32.402	22.280	1.00 22.13	A
	MOTA	1423	0	SER A	250		32.828	21.511	1.00 22.77	A
50	MOTA	1424	N	PRO A			33.029	23.425	1.00 22.23	A
	MOTA	1425	CD	PRO A	251	45.163	32.684	24.433	1.00 22.97	A
	ATOM	1426	CA	PRO I	251	46.893	34.254	23.800	1.00 22.52	Α
	ATOM	1427	CB	PRO A	251		34.650	25.127	1.00 23.06	A
	MOTA	1428	CG	PRO A	251	45.726	33.329	25.676	1.00 22.55	A
55	ATOM	1429	C	PRO A	251	48.414	34.115	23.907	1.00 22.15	A
	MOTA	1430	0	PRO A	251	49.143	35.047	23.563	1.00 22.62	, A
	MOTA	1431	N	GLU A	252	48.901	32.966	24.367	1.00 20.69	A
	ATOM	1432	CA	GLU A	A 252		32.772	24.500	1.00 21.40	A
	ATOM	1433	CB	GLU A	A 252	50.673	31.382	25.071	1.00 20.59	A

	MOTA	1434	CG	GLU	A	252	49.993	30.232	24.352	1.00	21.91	A
	MOTA	1435	CĎ	GLU	A	252	48.691	29.822	25.014	1.00	21.51	A
	MOTA	1436	OE1	GLU	Α	252	47.989	30.707	25.550	1.00	21.46	A
	MOTA	1437	OE2	GLU	A	252	48.367	28.613	24.993	1.00	20.23	. А
5	MOTA	1438	C	GLU	A	252	51.071	32.970	23.167	1.00	22.99	, A
	ATOM	1439	0	GLU	A	252	52.191	33.480	23.136	1.00	23.17	A
	ATOM	1440	N	LEU			50.441	32.576	22.064	1.00	23.00	A
	ATOM	1441	CA	LEU	A	253	51.068	32.753	20.758	1.00	25.62	A
	ATOM	1442	CB	LEU	Α	253	50.277	32.029	19.669	1.00	26.75	A
10	ATOM	1443	CG	LEU	А	253	50.743	30.620	19.296	1.00	31.87	A
	ATOM	1444	CD1	LEU	Α	253	50.433	29.651	20.422	1.00	31.81	A
	ATOM	1445	CD2	LEU	Α	253	50.044	30.179	18.015	1.00	31.86	A
	ATOM	1446	С	LEU	Α	253	51.201	34.228	20.371	1.00	26.94	· A
	MOTA	1447	0	LEU	A	253	52.107	34.601	19.626	1.00	27.09	A
15	ATOM	1448	N	LEU	A	254	50.297	35.059	20.877	1.00	25.83	A
	ATOM	1449	CA	LEU	Α	254	50.297	36.485	20.564	1.00	27.26	A
	MOTA	1450	CB	LEU	Α	254	48.858	37.006	20.564	1.00	25.84	A
	ATOM	1451	CG	LEU	Α	254	47.882	36.290	19.621	1.00	24.69	A
	ATOM	1452	CD1	LEU	Α	254	46.459	36.724	19.932	1.00	23.64	A
20	ATOM	1453	CD2	LEU	Α	254	48.236	36.597	18.177	1.00	24.24	A
	ATOM	1454	С	LEU	Α	254	51.134	37.314	21.537	1.00	30.62	A
	ATOM	1455	0	LEU	Α	254	51.633	38.383	21.187	1.00	32.35	· А
	ATOM	1456	N	THR-	Α	255	51.292	36.821	22.758	1.00	32.47	A
	MOTA	1457	CA	THR	Α	255	52.056	37.547	23.759	1.00	36.70	A
25	ATOM	1458	CB	THR	Α	255	51.368	37.478	25.127	1.00	34.51	A
	MOTA	1459	OG1	THR	Α	255	51.188	36.106	25.494	1.00	35.49	A
	ATOM	1460	CG2	THR	A	255	50.013	38.166	25.077	1.00	33.40	A
	ATOM	1461	С	THR	Α	255	53.477	37.035	23.910	1.00	40.09	A
	ATOM	1462	0	THR	Α	255	54.430	37.793	23.772	1.00	43.69	A
30	MOTA	1463	N	GLU	Α	256 °	53.617	35.747	24.189	1.00	44.77	Α.
	ATOM	1464	CA	GLU	Α	256	54.932	35.144	24.382	1.00	49.15	A
	MOTA	1465	СВ	GLU	Α	256 ·	54.866	34.143	25.534	1.00	51.24	A
	ATOM	1466	CG	GLU	Α	256 .	54.514°	34.786	26.862	1.00	56.03	A
	MOTA	1467	CD	GLU	A	256	54.053	33.780	27.893	1.00	58.83	A
35	MOTA	1468	OE1	GLU	Α	256	54.766	32.776	28.107	1.00	62.13	A
	ATOM	1469	OE2	GLU	Α	256	52.979	33.996	28.494	1.00	60.34	A
	ATOM	1470	С	GLU	Α	256	55.475	34.456	23.137	1.00	50.09	A
	ATOM	1471	0	GLU	Α	256	56.616	33.995	23.127	1.00	50.42	A
	ATOM	1472	N	LYS	Α	257	54.658	34.389	22.090	1.00	51.21	A
40	ATOM	1473	CA	LYS	Α	257	55.064	33.746	20.845	1.00	51.22	A
	ATOM	1474	CB	LYS	Α	257	56.244	34.502	20.227	1.00	53.28	A
	MOTA	1475	CG	LYS	Α	257	56.558	34.125	18.790	1.00	55.19	A
	ATOM	1476	CD	LYS	Α	257	57.709	34.961	18.253	1.00	57.52	A
	ATOM	1477	CE	LYS	Α	257	57.952	34.694	16.777	1.00	58.52	A
45	ATOM	1478	NZ	LYS	Α	257	58.290	33.268	16.515	1.00	60.88	A
	MOTA	1479	С	LYS			55.467	32.302	21.138	1.00	50.74	A
	ATOM	1480	0	LYS	A	257 [°]	56.432	31.790	20.577	1.00	52.26	· A
	MOTA	1481	N	SER	Α	258	54.721	31.654	22.027	1.00	48.07	A
	MOTA	1482	CA	SER	Α	258	54.999	30.273	22.402	1.00	46.87	A
50	ATOM	1483	CB	SER			55.590	30.229	23.812	1.00	48.88	A
	ATOM	1484	OG	SER			54.741	30.892	24.734	1.00	53.14	A
	ATOM	1485	C	SER	A	258	53.735	29.415	22.342	1.00	44.07	A
	ATOM	1486	0	SER			52.617	29.932	22.417	1.00	44.17	A
	ATOM	1487	N	ALA			53.917	28.105	22.204	1.00	38.30	A
55	ATOM	1488	CA	ALA			52.793	27.180	22.127	1.00	34.73	A
	ATOM	1489	CB	ALA			52.551	26.779	20.684		34.16	A
	ATOM	1490	C	ALA			53.042	25.940	22.977	1.00	32.34	A
	ATOM	1491	0	ALA			54.172	25.459	23.086	1.00	31.81	A
	ATOM	1492	N	CYS			51.975	25.428	23.579		28.58	A

	ÄTOM	1493	CA	CYS	A 2	60		52.056	24.244	24.425	1.00 26.27	A
	MOTA	1494	CB	CYS				52.183	24.654	25.892	1.00 26.53	Α.
	MOTA	1495	SG	CYS	A 2	60		50.846	25.739	26.469	1.00 32.91	Α
	ATOM	1496	С	CYS	A 2	60		50.786	23.435	24.224	1.00 22.83	A
5	MOTA	1497	0	CYS	A 2	60		49.892	23.856	23.495	1.00 22.14	A
	MOTA	1498	N	LYS	A 2	61		50.706	22.277	24.868	1.00 20.02	A
	ATOM	1499	CA	LYS	A 2	61		49.526	21.434	24.744	1.00 20.65	A
	MOTA	1500	CB	LYS	A 2	61		49:619	20.243	25.696	1.00 23.28	A
	MOTA	1501	CG	LYS	A 2	61		50.716	19.253	25.347	1.00 27.44	A
10	MOTA	1502	CD	LYS	A 2	61		50.732	18.117	26.350	1.00 29.98	· A
	MOTA	1503	CE	LYS	A 2	61		51.922	17.203	26.134	1.00 32.34	A
	ATOM	1504	NZ	LYS	A 2	61		51.940	16.121	27.153	1.00 33.28	A
	MOTA	1505	С	LYS	A 2	61		48.268	22.229	25.062	1.00 19.20	A
	MOTA	1506	0	LYS	A 2	61		47.253	22.092	24.387	1.00 18.08	A
15	MOTA	1507	N	SER	A 2	62		48.358	23.068	26.089	1.00 16.92	A
	MOTA	1508	CA	SER	A 2	62		47.235	23.883	26.534	1.00 18.13	A
	ATOM	1509	CB	SER	A 2	62		47.644	24.698	27.770	1.00 18.27	A
	MOTA	1510	OG	SER	A 2	62	- 0	46.517	25.258	28.421	1.00 22.53	A
	ATOM	1511	С	SER	A 2	62		46.736	24.811	25.424	1.00 16.77	A
20	ATOM	1512	0	SER	A 2	62		45.591	25.254	25.450		. A
	MOTA	1513	N	SER				47.595	25.118	24.456	1.00 16.44	A
	MOTA	1514	CA	SER	A 2	263		47.175	25.970	23.347	1.00 16.89	A
	MOTA	1515	CB	SER	A 2	263		48.340	26.228	22.382	1.00 18.49	A
	ATOM	1516	OG	SER	A 2	63		49.402	26.909	23.031	1.00 22.10	A
25	ATOM-	1517	С	SER	A 2	263		46.040	25.257	22.612	1.00 17.79	A
	ATOM	1518	0	SER	A 2	263		45.099	25.898	22.148	1.00 17.57	A
	ATOM	1519	N	ASP	A 2	264		46.119	23.928	22.517	1.00 16.30	A
	ATOM	1520	CA	ASP	A 2	264		45.069	23.166	21.836	1.00 16.72	A
	ATOM	1521	CB	ASP				45.483'		21.620	1.00 15.92	· A
30	ATOM	1522	CG	ASP	A 2	264		46.544	21.539	20.548	1.00 17.93	A
	ATOM	1523		ASP				46.642	22.412	19.661	1.00 16.78	A
	MOTA	1524	OD2	ASP	A 2	264		47.265	20.515	20.579	1.00 16.64	A
	MOTA	1525	C.	ASP				43.773	23.194	22.646	1.00 17.67	A
	MOTA	1526	0	ASP				42.681	23.197	22.076	1.00 18.27	A
35	MOTA	1527	N	LEU				43.898	23.205	23.974	1.00 15.49	
	MOTA	1528	CA	LEU				42.730	23.232	24.849	1.00 14.75	
	ATOM	1529	CB	LEU				43.147	23.038	26.313	1.00 11.38	A A
	MOTA	1530	CG	LEU				43.711	21.641	26.621	1.00 14.04 1.00 13.96	
	MOTA	1531		LEU				44.249	21.579	28.052	•	
· 40	ATOM	1532		LEU			•	42.619	20.603	26.416	1.00 11.62 1.00 15.13	
	MOTA	1533	С	LEU				41.999	24.557	24.675	1.00 15.13	
	MOTA	1534	0	LEU				40.777	24.620	24.785	1.00 16.73	
	MOTA	1535	N	TRP				42.746	25.622	24.405	1.00 16.08	
	MOTA	1536	CA	TRP				42.118	26.918	24.184	1.00 10.30	A
45	ATOM	1537	СВ	TRP				43.176	28.015	24.023	1.00 17.28	
	ATOM	1538	CG	TRP			•	42.618	29.326	23.521	1.00 20.07	
	ATOM	1539.		TRP				42.313	30.490	24.301	1.00 20.07	
	MOTA	1540		TRP				41.782	31.459	23.417	1.00 20.40	A
	MOTA	1541		TRĖ				42.435	30.810	25.660 22.231	1.00 20.68	
50	ATOM	1542		TRP				42.270	29.631	22.231	1.00 19.61	
	ATOM	1543		TRP				41.769	30.908	23.850	1.00 19.81	
	ATOM	1544		TRP				41.372	32.727	26.091	1.00 20.30	
	ATOM	1545		TRP				42.026	32.073	25.185	1.00 19.43	
۔ م	ATOM	1546		TRP				41.501	33.015	22.913	1.00 20.71	
55	ATOM	1547	C	TRP				41.284	26.795	22.863	1.00 17.22	
	ATOM	1548	0	TRP				40.139	27.240	21.886	1.00 17.50	
	ATOM	1549	N	ALA				41.863	26.181	20.626	1.00 17.30	
	ATOM	1550	CA	ALA				41.155	25.990	19.621	1.00 14.28	
	ATOM	1551	CB	ALA	A.	201		42.050	25.290	13.021	1.00 13.20	A

	ATOM	1552	С	ALA A	267	39.901	25.159	20.891	1.00 16.28	A
	ATOM	1553 [°]	0	ALA A	267	38.835	25.436	20.346	1.00 16.46	A
	ATOM	1554	N	LEU A	268	40.031	24.144	21.739	1.00 16.57	A
	ATOM	1555	CA	LEU A	268	38.890	23.299	22.084	1.00 17.03	A
5	ATOM	1556	CB	LEU A	268	39.292	22.260	23.139	1.00 15.35	A
	ATOM	1557	CG	LEU A	268	38.158	21.429	23.754	1.00 19.00	A
	ATOM	1558		LEU A		37.505	20.578	22.678	1.00 16.17	A
	ATOM	1559		LEU A		38.718	20.537	24.881	1.00 17.49	A
	ATOM	1560	C	LEU A		37.766	24.179	22.628	1.00 15.72	· A
10	ATOM	1561	ō	LEU A		36.603	24.031	22.247	1.00 15.28	A
	ATOM	1562	N	GLY A		38.119	25.099	23.520	1.00 14.34	A
	ATOM	1563	CA	GLY A		37.124	25.989	24.092	1.00 13.39	A
	ATOM	1564	C	GLY A		36.406	26.808	23.031	1.00 14.94	A
	ATOM	1565	o	GLY A		35.193	27.014	23.114	1.00 14.76	A
15	ATOM	1566	N	CYS A		37.146	27.279	22.030	1.00 13.86	A
13	ATOM	1567	CA	CYS A		36.539	28.061	20.958	1.00 16.80	A
	ATOM	1568	CB	CYS A		37.611	28.634	20.023	1.00 15.97	A
	ATOM	1569	SG	CYS A		38.751	29.810	20.780	1.00 20.48	A
	ATOM	1570	C	CYS A		35.598	27.175	20.140	1.00 17.50	A
20	ATOM	1571	0	CYS A		34.516	27.604	19.741	1.00 17.30	A
20		1572	Ŋ	ILE A		36.022	25.939	19.887	1.00 16.99	A
	MOTA	1572	CA	ILE A		35.221	25.004	19.104	1.00 16.66	A
	MOTA	1574	CB	ILE A		36.038	23.741	18.778	1.00 16.53	A
	ATOM	1575		ILE A		35.155	22.694	18.102	1.00 16.33	. A
25	ATOM					37.222	24.129	17.882	1.00 15.59	A
25	ATOM	1576	CG1	ILE A		38.239	23.018	17.690	1.00 13.39	A
	ATOM	1577	CD1	ILE A		33.920	24.626	19.809	1.00 14.88	A
	ATOM	1578	С						1.00 10.74	A
	ATOM	1579	0	ILE A		32.865	24.576 24.357	19.179 21.111	1.00 17.12	A
20	ATOM	1580	N	ILE A		33.990 32.785		21.862	1.00 18.13	A
30	ATOM	1581	CA	ILE A		33.097	24.021 23.747	23.346	1.00 17.77	A
	ATOM	1582	CB	ILE A				24.152	1.00 17.77	A
	ATOM.	1583		ILE A		31.796	23.666		1.00 17.36	A
	ATOM	1584	CG1			33.877	22.437 22.217	23.481 24.886	1.00 19.55	A
25	ATOM	1585		ILE A		34.446			1.00 18.04	A
35	ATOM	1586	С	ILE A		31.824	25.207	21.776 21.554	1.00 19.31	A
	ATOM	1587	0	ILE A		30.624	25.037		1.00 20.44	A
	ATOM	1588	N	TYR A		32.362	26.409	21.947	1.00 18.32	A
	ATOM	1589	CA	TYR A		31.553	27.615	21.881	1.00 20.48	A
40	ATOM	1590	CB	TYR A		32.418	28.847	22.162		A
40	ATOM	1591	CG ·			31.663	30.161	22.125	1.00 20.26	A
	ATOM	1592	CD1			31.229	30.709	20.916 20.880	1.00 20.67	A
	ATOM	1593	CE1			30.536	31.917 30.857		1.00 20.36	A
	ATOM	1594	CD2			31.383		23.302 23.280		A
45	ATOM	1595	CE2	TYR A		30.691	32.062		1.00 20.62	
45	ATOM	1596	CZ	TYR A		30.271	32.587	22.067	1.00 21.15	A
	ATOM	1597	OH	TYR A		29.588	33.776	22.049	1.00 21.86	A
	ATOM	1598	С	TYR A		30.902	27.730	20.507	1.00 21.54	A
	ATOM	1599	0	TYR A		29.719	28.049	20.401	1.00 22.80	A
~ 0	ATOM	1600	N	GLN A		31.676	27.454	19.461	1.00 21.05	A
50	ATOM	1601	CA	GLN A		31.176	27.538	18.095	1.00 21.48	A
	ATOM	1602	CB	GLN A		32.323	27.341	17.097	1.00 21.41	A
	ATOM	1603	CG	GLN A		31.934	27.596	15.645	1.00 23.15	A
	ATOM	1604	CD	GLN A		33.131	27.588	14.706	1.00 24.80	A
	ATOM	1605		GLN A		34.276	27.446	15.139	1.00 22.51	A
55	MOTA	1606	NE2			32.870	27.750	13.413	1.00 22.96	A
	ATOM	1607	C -	GLN A		30.076	26.517	17.828	1.00 21.51	A
	ATOM	1608	0	GLN A		29.123	26.806	17.108	1.00 20.50	. A
	MOTA	1609	N	LEU A		30.207	25.324	18.403	1.00 21.44	A
	ATOM	1610	CA	LEU A	275	29.196	24.282	18.208	1.00 20.95	A
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	MOTA	1611	CB	LEU A	A 27!	29.64	5 22.958	18.846	1.00 19.11	A
	ATOM	1612	CG	LEU A	A 27	30.77	5 22.182	18.159	1.00 21.43	`A
	ATOM	1613	CD1	LEU A	A 27!	31.11		18.963	1.00 17.64	A
	ATOM	1614	CD2	LEU Z	A 275	30.34	2 21.795	16.754	1.00 20.34	A
5	ATOM	1615	С	LEU Z	A 275	27.86	0 24.697	18.815	1.00 21.32	A
	ATOM	1616	Ó	LEU A				18.229	1.00 19.75	A
	ATOM	1617	N	VAL A				19.987	1.00 19.10	A
	ATOM	1618	CA	VAL A				20.702	1.00 22.47	A
	ATOM	1619	CB	VAL A				22.217	1.00 20.87	A
10	ATOM	1620		VAL A				22.957	1.00 19.68	A
20	ATOM	1621	CG2					22.766	1.00 19.43	A
	ATOM	1622	C	VAL 2				20.211	1.00 23.89	A
	ATOM	1623	Õ	VAL A				20.070	1.00 24.90	A
	ATOM	1624	N	ALA A				19.965	1.00 24.56	A
15	ATOM	1625	CA	ALA A				19.518	1.00 24.72	A
13	ATOM	1626	CB	ALA A				19.999	1.00 24.36	A
	ATOM	1627	C	ALA Z				18.005	1.00 25.76	A
•	ATOM	1628	Ö	ALA A			•	17.502	1.00 25.70	A
	ATOM	1629	N	GLY A				17.280	1.00 25.13	Ā
20	ATOM	1630	CA	GLY A				15.834	1.00 25.13	A
20	ATOM	1631	C	GLY A			•	15.231	1.00 25.50	A
		1632	0	GLY A				14.015	1.00 28.17	A
	MOTA	1633	N	LEU A				16.086	1.00 28.17	A
	ATOM			LEU A				15.656	1.00 24.44	A
25	ATOM	1634	CA	LEU A				15.500	1.00 25.21	A
25	MOTA	1635	CB	LEU A				14.490	1.00 23.78	A
	MOTA	1636	CG	LEU A					1.00 26.60	A
	MOTA	1637		LEU A				14.684 13.071	1.00 26.50	A
	MOTA	1638		LEU A				16.687	1.00 28.32	A
30	MOTA	1639	C	LEU A				17.882	1.00 23.47	A
30	MOTA	1640	O N	PRO A				16.236	1.00 23.35	A
	ATOM ATOM	1641 1642	CD	PRO I				14.855	1.00 23.35	A
	ATOM ATOM	1643	CA	PRO I				17.189	1.00 23.81	A
	ATOM	1644	CB	PRO A				16.282	1.00 23.01	A
35	ATOM	1645	CG	PRO I				15.073	1.00 24.89	A
33	ATOM	1646	C	PRO A				18.137	1.00 22.69	A
	MOTA	1647	Ö	PRO A				17.788	1.00 22.11	A
	ATOM	1648	N	PRO A				19.345	1.00 23.06	A
	ATOM	1649	CD	PRO A				19.734	1.00 21.37	A
40	ATOM	1650	CA	PRO A				20.395	1.00 23.67	A
40	ATOM	1651	CB	PRO A				21.509	1.00 24.89	. A
	ATOM	1652	CG	PRO A				21.219	1.00 25.24	
	ATOM	1653	C	PRO A				20.017	1.00 23.75	A
	ATOM	1654	Ö	PRO A				20.317	1.00 21.02	A
45	ATOM	1655	N	PHE A				19.379	1.00 22.17	A
73	ATOM	1656	CA	PHE A				18.998	1.00 23.16	A
	ATOM	1657	CB	PHE A				19.406	1.00 21.01	A
•	ATOM	1658	CG	PHE A				20.822	1.00 22.66	A
	ATOM	1659		PHE I				21.888	1.00 20.06	A
50	ATOM	1660		PHE F				21.093	1.00 20:72	A
50	ATOM	1661		PHE F				23.206	1.00 22.66	A
	ATOM	1662		PHE A				22.405	1.00 20.97	A
	ATOM	1663	CZ	PHE A				23.466	1.00 19.58	A
	ATOM	1664	C	PHE F				17.503	1.00 24.39	A
55	ATOM	1665	o	PHE A				16.694	1.00 25.80	A
	ATOM	1666	N	ARG A				17.142	1.00 24.99	A
	ATOM	1667	CA	ARG F				15.741	1.00 26.33	A
	ATOM	1668	CB	ARG F				15.316	1.00 28.91	A
	ATOM	1669	CG	ARG A				15.724	1.00 30.27	A
			-5			55.65				

	ATOM	1670	CD	ARG A	283	31.904	35.493	15.188	1.00 33.36	A
	MOTA	1671	NE	ARG A	283	30.890	36.392	15.733	1.00 32.76	. А
	MOTA	1672	CZ	ARG A	283	30.372	36.287	16.952	1.00 34.79	A
	MOTA	1673	NH1	ARG A	283	30.767	35.317	17.768	1.00 35.77	Α
5	MOTA	1674	NH2	ARG A	283	29.458	37.156	17.359	1.00 36.12	A
•	ATOM	1675	С	ARG A		35:328	39.096	15.544	1.00 26.47	A
	ATOM	1676	O	ARG A		35.029	39.888	16.438	1.00 26.28	A
	ATOM	1677	N	ALA A	284	35.818	39.486	14.373	1.00 26.70	A
	ATOM	1678	CA	ALA A		36.033	40.899	14.079	1.00 27.84	A
10	ATOM	1679	CB	ALA A		37.188	41.442	14.914	1.00 26.24	A
10	ATOM	1680	C	ALA A		36.327	41.077	12.602	1.00 28.35	A
	ATOM	1681	Ö	ALA A		36.560	40.101	11.891	1.00 29.91	A
	ATOM	1682	N	GLY A		36.332	42.329	12.153	1.00 29.29	A
	ATOM	1683	CA	GLY A		36.577	42.631	10.753	1.00 29.52	A
15	ATOM	1684	C	GLY A		37.893	42.156	10.168	1.00 30.12	A
13		1685	Ö	GLY A		37.974	41.862	8.976	1.00 30.60	A
	ATOM	1686	N	ASN A			42.097	10.983	1.00 28.49	A
	ATOM	1687	CA	ASN A			41.644	10.489	1.00 26.71	· A
	MOTA	1688		ASN A			42.825	9.945	1.00 26.71	A
00	ATOM		CB	ASN A			43.900	10.990	1.00 27.83	A
20	ATOM	1689	CG				43.631	12.049	1.00 27.84	A
	MOTA	1690		ASN A			45.131	10.685	1.00 27.04	A
	ATOM	1691		ASN A			40.924	11.584	1.00 25.93	A
	MOTA	1692	С				40.924	12.723	1.00 25.66	A
0.5	ATOM	1693	0.	ASN A			40.831	11.239	1.00 23.00	A
25	MOTA	1694	N	GLU A		42.162	39.662	12.206	1.00 27.59	A
,	MOTA	1695	CA	GLU A		42.965		11.510	1.00 27.33	A
	ATOM	1696	CB	GLU Z			38.985		1.00 30.17	A
	ATOM	1697	CG	GLU A		43.776	37.632	10.931	1.00 38.21	A
	ATOM	1698	CD	GLU A			36.998	10.140	1.00 41.80	A
30	MOTA	1699		GLU A			37.036	10.608	1.00 45.00	A
	ATOM	1700		GLU A			36.449	9.052	1.00 45.22	A
	ATOM	1701	С	GLU Z			40.485	13.383		A
	ATOM	1702	0	GLU Z			40.030	14.521	1.00 26.41 1.00 23.04	A
	ATOM	1703	N	TYR A			41.685	13.122	1.00 23.04	A
35	MOTA	1704	CA	TYR A			42.528	14.205	1.00 22.34	A
	ATOM	1705	CB	TYR A			43.913	13.691		A
	ATOM	1706	CG	TYR A			44.858	14.805	1.00 21.07	A
	ATOM	1707		TYR A			44.762	15.405	1.00 21.23	A
	ATOM	1708	CE1				45.588	16.475	1.00 20.43	A
40	ATOM	1709		TYR A			45.809	15.302	1.00 22.32	A
	ATOM	1710		TYR A		•		16.373	1.00 23.28	A
	ATOM	1711	CZ		A 288		46.518	16.953	1.00 22.30	A
	ATOM	1712	ОН		288		47.313	18.024	1.00 23.18	A
	ATOM	1713	С		1 288		42.698	15.288	1.00 21.38	A
45	ATOM	1714	0	TYR A			42.616	16.473		
	ATOM	1715	N	LEU Z			42.939	14.874	1.00 21.88	A
	ATOM	1716	CA	LEU A			43.130	15.811	1.00 21.98	A
	ATOM	1717	CB	LEU A			43.673	15.078	1.00 22.90	A
	ATOM	1718	CG	LEU A			45.130	14.601	1.00 26.52	A
50	MOTA	1719		LEU A			45.436	13.696	1.00 26.55	A
	ATOM	1720		LEU I			46.071	15.807	1.00 23.13	A
	ATOM	1721	С	LEU A			41.849	16.560	1.00 21.24	A
	ATOM	1722	0		1 289		41.897	17.715	1.00 20.72	A
	MOTA	1723	N		A 290		40.708	15.900	1.00 19.62	A
55	ATOM	1724	CA		1 290		39.433	16.533	1.00 18.54	A
	ATOM	1725	CB		A 290		38.281	15.509	1.00 18.52	A
	ATOM	1726		ILE A			36.934	16.234	1.00 17.63	. A
	ATOM	1727		ILE 2			38.429	14.545	1.00 18.88	. A
	ATOM	1728	CD1	ILE A	1 290	39.421	37.483	13.357	1.00 19.81	A

							•				
	ATOM	1729	С	ILE A	290	41.5	78 39.1	6.7 17.618	1.00	19.09	A
	ATOM	1730	0	ILE A	290	41.2	36 38.7	88 18.737		18.20	Α
	MOTA	1731	N	PHE A	291	42.8	39.3°	76 17.286		18.76	A
	ATOM	1732	CA	PHE A	291	43.9	25 39.1	56 18.247	1.00	20.75	A
5	ATOM	1733	CB	PHE A	291	45.2	86 39.43	34 17.606	1.00	20.71	· A
	ATOM	1734	CG	PHE A	291	45.6	38.48	30 16.503	1.00	22.92	A
	ATOM	1735	CD1	PHE A		45.0	65 37.2	14 16.443	1.00	22.98	A
	ATOM	1736	CD2	PHE A	291	46.5				22.91	A
	ATOM	1737		PHE A		45.4				24.51	A
10	ATOM	1738		PHE A		46.9				25.54	A
	ATOM	1739	CZ	PHE A		46.3	- "			23.29	A
	ATOM	1740	C	PHE A		43.7				21.72	A
	ATOM	1741	ō	PHE A		43.9				22.32	· A
	ATOM	1742	N	GLN A		43.2				23.27	A
15	ATOM	1743	CA	GLN A		43.0				24.01	A
10	ATOM	1744	СВ	GLN A		42.5				25.77	A
	MOTA	1745	CG	GLN A		42.5				28.45	A
	MOTA	1746	CD	GLN A		42.4				29.83	A
	ATOM	1747		GLN A		41.5				27.16	A
20	ATOM	1748		GLN A		43.4				27.61	A
20	ATOM	1749	C	GLN A		42.0				22.97	A
	ATOM	1750	ō	GLN A		42.2				21.64	A
	ATOM	1751	N	LYS A		40.9				21.82	A
	ATOM	1752	CA	LYS A		39.8				22.18	A
25	ATOM	1753	CB	LYS A		38.6				22.69	A
23	ATOM	1754	CG	LYS A		37.9				25.78	A
	ATOM	1755	CD	LYS A		36.6	•			27.88	A
	ATOM	1756	CE	LYS A		35.8				30.85	A
	ATOM	1757	NZ	LYS A		34.6				32.98	A
30	ATOM	1758	C	LYS A		40.3				21.20	A
50	ATOM	1759	ŏ	LYS A	•	40.0				22.01	A
	ATOM	1760	N	ILE A		41.2				19.91	A
	ATOM	1761	CA	ILE A		41.7		•		20.28	A
	ATOM	1762	CB	ILE A		42.6				18.98	A
35	ATOM	1763	CG2			43.4				17.70	A
33	ATOM	1764		ILE A		41.7				17.93	A
	ATOM	1765	CD1			42.4				16.21	A
	ATOM	1766	C	ILE A		42.6				21.94	· A
	ATOM	1767	ō	ILE A		42.3				20.86	A
40	ATOM	1768	N	ILE A		43.6				21.88	A
	ATOM	1769	CA	ILE A		44.4			1.00		A
	ATOM	1770	CB	ILE A		45.6				23.93	A
	ATOM	1771	CG2	ILE A		46.5				24.61	A
	ATOM	1772	CG1			45.1			1.00		A
45	ATOM	1773	CD1			46.3				26.69	A
	MOTA	1774	C	ILE A		43.7			1.00		A
	ATOM	1775	ō	ILE A						24.76	A
	ATOM	1776	N	LYS A		42.5			1.00		A
	ATOM	1777	CA	LYS A		41.7			1.00		A
50	ATOM	1778	CB	LYS A		41.1			1.00		A
	ATOM	1779	CG	LYS A		42.2			1.00		A
	ATOM	1780	CD	LYS A		41.6			1.00		A
	ATOM	1781	CE	LYS A		41.0			1.00		A
	ATOM	1782	NZ	LYS A		40.5			1.00		A
55	ATOM	1783	C	LYS A		40.5			1.00		A
	ATOM	1784	Ö	LYS A		39.7			1.00		A
	ATOM	1785	N	LEU A		40.5			1.00		A
	ATOM	1786	CA	LEU A		39.5			1.00		A
	ATOM	1787	CB	LEU A		39.6			1.00		A
	·										

	ATOM	1788	CG	LEU A	.297	38.766	36.068	28.460	1.00 26.43	A
	ATOM	1789		L LEU A		39.238	34.852			
	ATOM	1790		LEU A				27.646	1.00 26.70	A
						38.856	35.777	29.951	1.00 24.84	A
_	MOTA	1791	С	LEU A		38.151	38.459	26.467	1.00 25.11	A
5	MOTA	1792	0	LEU A		37.261	38.378	27.309	1.00 25.28	A
	ATOM	1793	N	GLU À	. 298	38.007	39.127	25.331	1.00 24.98	A
	ATOM	1794	CA	GLU A	298	36.786	39.847	25.023	1.00 25.31	A
	ATOM	1795	CB	GLU A	298	37.143	41.139	24.291	1.00 27.13	A
	ATOM	1796	CG	GLU A		35.991	42.092	24.108	1.00 31.28	
10	ATOM	1797	CD	GLU A		36.419				A
10							43.362	23.410	1.00 34.40	A
	ATOM	1798		GLU A		37.348	44.027	23.918	1.00 35.90	, . A
	MOTA	1799		GLU A		35.832	43.693	22.359	1.00 36.16	A
	ATOM	1800	С	GLU A		35.766	39.057	24.207	1.00 23.79	A
	ATOM	1801	0	GLU A	298	35.832	39.017	22.979	1.00 24.35	A
15	ATOM	1802	N	TYR A	299	34.825	38:427	24.902	1.00 23.45	A
	ATOM	1803	CA	TYR A		33.760	37.663	24.265	1.00 23.98	
	ATOM	1804	CB	TYR A		34.264	36.304	23.755	1.00 20.13	
	ATOM	1805	CĠ	TYR A		34.348				A
							35.233	24.828	1.00 21.17	A
00	ATOM	1806		TYR A		35.336	35.279	25.810	1.00 19.32	A
20	ATOM	1807		TYR A		35.389	34.332	26.826	1.00 19.30	A
	ATOM	1808	CD2	TYR A	299	33.410	34.201	24.888	1.00 18.96	A
	MOTA	1809	CE2	TYR A	299	33.456	33.243	25.907	1.00 19.41	A
	ATOM	1810	CZ	TYR A	299	34.449	33.321	26.870	1.00 18.79	A
	ATOM	1811	ОН	TYR A	299	34.511	32.401	27.881	1.00 18.77	A
25	MOTA	1812	С	TYR A			.37.437	25.331	1.00 25.20	A
	ATOM	1813	ō	TYR A		32.942	37.681	26.506	1.00 26.46	A
	ATOM	1814	N	ASP A		31.522				
							36.981	24.927	1.00 26.94	A
•	ATOM	1815	CA	ASP A		30.467	36.710	25.891	1.00 30.60	A
	ATOM	1816	CB	ASP A		29.665	37.981	26.179	1.00 35.86	A
30	ATOM	1817	CG	ASP A		29.228	38.687	24.923	1.00 42.04	A
	ATOM	1818	OD1	ASP A	300	28.450	38.088	24.149	1.00 45.98	A
	MOTA	1819	OD2	ASP A	300	29.666	39.840	24.707	1.00 45.69	Α
	ATOM	1820	С	ASP A	300	29.564	35.608	25.363	1.00 29.26	A
	ATOM	1821	0	ASP A	300	29.590	35.299	24.172	1.00 28.64	Α
35	ATOM	1822	N	PHE A		28.778	35.011	26.253	1.00 28.96	A
	ATOM	1823	CA	PHE A		27.884	33.924	25.871	1.00 30.48	A
	ATOM	1824	CB	PHE A		27.818	32.854			
								26.968	1.00 29.17	A
	ATOM	1825	CG	PHE A		29.147	32.279	27.356	1.00 29.29	Α
	ATOM	1826		PHE A		29.978	32.949		1.00 27.31	A
40	ATOM	1827		PHE A		29.560	31.050	26,845	1.00 27.89	· A
	ATOM	1828	CE1	PHE A	301	31.205	32.403	28.625	1.00 28.83	A
	ATOM	1829	CE2	PHE A	301	30.781	30.498	27.217	1.00 28.05	Α
	ATOM	1830	CZ	PHE A	301	31.605	31.175	28.110	1.00 28.27	A
	ATOM	1831	С	PHE A		26.459	34.384	25.619	1.00 32.20	A
45	ATOM		ō	PHE A		25.946	35.261	26.317	1.00 32.36	A
	ATOM	1833	N	PRO A		25.798	33.804	24.607	1.00 32.30	
	ATOM	1834		PRO A						A
			CD			26.313	32.943	23.529	1.00 34.04	A
	ATOM	1835	CA	PRO A		24.415	34.199	24.341	1.00 35.24	A
	ATOM	1836	CB	PRO A		24.144	33.608	22.959	100 34.01	A
50	ATOM	1837	CG	PRO A		25.041	32.413	22.921	1.00 35.48	Α
	ATOM	1838	C	PRO A	302	23.567	33.561	25.444	1.00 37.39	Α
	ATOM	1839	O	PRO A	302	23.935	32.518	25.986	1.00 38.49	·- A
	ATOM	1840	N	ALA A		22.447	34.188	25.783	1.00 39.36	A
	ATOM	1841	CA	ALA A		21.572	33.692	26.843	1.00 40.65	A
55	ATOM	1842	CB	ALA A		20.280	34.506	26.862	1.00 41.66	
-	ATOM	1843	С				32.197			A
				ALA A		21.238		26.814	1.00 41.25	A
	ATOM	1844	0	ALA A		21.253	31.537	27.854	1.00 43.16	A
	ATOM	1845	N	ALA A		20.945	31.665	25.631	1.00 41.04	A
	MOTA	1846	CA	ALA A	304	20.569	30.258	25.480	1.00 40.66	A

	ATOM	1847	CB	ALA	A	304		20.121	30.004	24.040	1.00 41.36	A
	MOTA	1848	C			304		21.628	29.223	25.876	1.00 39.61	A
	ATOM	1849	0	ALA	A	304		21.298	28.156	26.395	1.00 40.61	A
	ATOM	1850	N	PHE	Α	305		22.891	29.543	25.617	1.00 36.21	A
5	ATOM	1851	CA			305		24.022	28.662	25,909	1.00 32.08	A
	ATOM	1852	CB	PHE	A	305		25.259	29.519	26.187	1.00 29.46	A
	ATOM	1853	CG			305		26.536	28.917	25.690	1.00 28.15	A
	ATOM	1854		PHE				27.146	27.875	26.377	1.00 26.20	A
	ATOM	1855		PHE				27.127	29.386	24.521	1.00 27.05	A
10	ATOM	1856		PHE				28.330	27.308	25.908	1.00 26.92	A
	ATOM	1857		PHE				28.312	28.826	24.042	1.00 26.62	A
	ATOM	1858	CZ			305		28.914	27.786	24.737	1.00 26.61	A
	ATOM	1859	c			305		23.811	27.664	27.057	1.00 20.01	A
	ATOM	1860	Ö			305		23.518	28.051	28.187	1.00 30.03	A
15	ATOM	1861	N			306		23.964	26.378	26.758	1.00 31.31	A
10	ATOM	1862	CA			306	•	23.801	25.334	27.769	1.00 26.30	A
	ATOM	1863	CB			306		24.157	23.970	27.170	1.00 25.03	A
	ATOM	1864	CG			306		23.548	23.725	25.815	1.00 23.03	A
	ATOM	1865		PHE				22.170	23.723	25.622	1.00 27.24	A
20	ATOM	1866	•	PHE				24.350	23.386	24.728	1.00 27.84	A
20	ATOM	1867		PHE				21.601	23.603	24.726	1.00 27.84	A
	ATOM	1868		PHE				23.792	23.155	23.465	1.00 28.03	A
	ATOM \	1869	CZ			306		22.415	23.263	23.283	1.00 28.00	A
	ATOM	1870	C			306		24.711	25.652	28.961	1.00 26.23	A
25	ATOM	1871	0			306		25.927	25.775	28.811	1.00 25.23	A
23			N			307		24.125	25.775	30.163	1.00 25.53	A
	ATOM ATOM	1872 1873	CD			307		22.685	25.625	30.430	1.00 20.07	A
	ATOM	1874	CA			307		24.842	26.110	31.405	1.00 27.55	A
	ATOM	1875	CB			307		23.795	25.832	32.481	1.00 26.14	A
30	ATOM	1876	CG			307		22.531	26.250	31.803	1.00 27.86	A
50	ATOM	1877	C			307		26.145	25.355	31.659	1.00 27.50	Ā
	ATOM	1878	0			307		27.189	25.964	31.900	1.00 23.58	A
	ATOM	1879	Ŋ			308		26.085	24.031	31.620	1.00 22.05	A
	ATOM	1880	CA			308	•	27.274	23.232	31.867	1.00 23.91	A
35	ATOM	1881	CB			308		26.887	21.760	32.024	1.00 23.25	
33	ATOM	1882	CG			308		26.062	21.532	33.285	1.00 28.49	. A
	ATOM	1883	CD			308		25.618	20.093	33.466	1.00 20.43	A
	ATOM	1884	CE			308		24.760	19.973	34.722	1.00 33.12	A
	ATOM	1885	NZ	LYS				24.122	18.636	34.860	1.00 34.13	A
40	ATOM	1886	C	LYS				28.314	23.426	30.769	1.00 22.84	A
.0	ATOM	1887	ŏ	LYS				29.514	23.411	31.042	1.00 22.46	A
	ATOM	1888	N			309		27.861	23.621	29.534	1.00 21.59	A
	ATOM	1889	CA	ALA		309		28.792	23.848	28.432	1.00 20.02	A
	ATOM	1890	CB	ALA				28.056	23.856	27.106	1.00 18.80	A
45	ATOM	1891	ċ	ALA				29.481	25.191	28.662	1.00 21.41	A
	ATOM	1892	Ö	ALA				30.680	25.335	28.427	1.00 21.39	A
	ATOM	1893	N	ARG				28.717	26.179	29.121	1.00 21.39	A
	ATOM	1894	CA	ARG				29.290	27.494	29.388	1.00 22.02	A
	ATOM	1895	CB	ARG				28.213	28.479	29.854	1.00 22.39	A
50	ATOM	1896	CG	ARG				28.806	29.756	30.436	1.00 25.30	A
	ATOM	1897	CD	ARG				27.780	30.852	30.664	1.00 28.33	A
	ATOM	1898	NE	ARG				28.420	32.039	31.230	1.00 30.18	A
	ATOM	1899	CZ	ARG				27.901	33.263	31.203	1.00 32.07	A
	ATOM	1900		ARG				26.719	33.477	30.634	1.00 31.19	A
55	ATOM	1901		ARG				28.567	34.277	31.742	1.00 30.49	A
	ATOM	1902	С	ARG				30.376	27.388	30.458	1.00 21.65	. A
	ATOM	1903	Ö	ARG				31.464	27.949	30.311	1.00 20.36	A
	ATOM	1904	N	ASP				30.074	26.677	31.541	1.00 19.57	A
	ATOM	1905	CA	ASP				31.043	26.512	32.615	1.00 20.18	A

				•								
	ATOM	1906	CB	ASP	A 31	1	30.460	.25.649	33.739	1.00	.20.39	Α
	ATOM	1907	CG		A 31		31.439	25.446	34.881		23.35	
												A
	ATOM	1908	ODI	ASP	A 31	L	32.158	24.428	34.885	1.00	24.91	A
	ATOM	1909	OD2	ASP	A 31	1	31.500	26.312	35.776	1.00	26.96	Α
5	ATOM	1910	С	ASP			32.322	25.877	32.073		19.73	. A
-												
	MOTA	1911	0	ASP			33.422	26.289	32.439		19.30	A
	MOTA .	1912	N	LEU	A∙ 31	2	32.179	24.891	31.188	1.00	16.32	A
	MOTA	1913	CA	LEU	A 31	2	33.349	24.226	30.611	1.00	16.66	A
	ATOM	1914	CB	LEU			32.927	23.035	29.744			
• •											16.12	A
10	ATOM	1915	CG	LEU	A 31	2	34.050	22.320	28.974	1.00	14.73	A
	ATOM	1916	CD1	LEU	A 31	2	35.192	21.935	29.912	1.00	14.56	Α
	ATOM	1917	CD2	LEU	Δ 31	2	33.477	21.084	28.289	1 00	14.22	A
	ATOM	1918	C	LEU			34.181	25.189	29.774		16.61	A
	ATOM	1919·	0	LEU	А 31	2	35.402	25.241	29.910	1.00	16.20	A
15	ATOM	1920	N	VAL	A 31	3	33.515	25.949	28.908	1.00	16.20	A
	ATOM	1921	CA	VAL			34.207	26.907	28.058		15.37	A
	MOTA	1922	CB	VAL			33.216	27.648	27.130		16.42	A
	MOTA	1923	CG1	VAL	A 31	3	33.915	28.796	26.426	1.00	16.93	A
	ATOM	1924	CG2	VAL	A 31	3	32.644	26.672	26.103	1.00	17.88	A
20	ATOM	1925	C	VAL			34.960	27.923	28.911		17.39	A
20												
	MOTA	1926	0	VAL			36.093	28.294	28.591	1.00	18.00	A
	MOTA	1927	N	GLU	A 31	1	34.342	28.364	30.004	1.00	17.61	. A
	ATOM	1928	CA	GLU	A 31	1 ·	34.986	29.331	30.885	1.00	20.43	A
				GLU				29.816				
	MOTA	1929	СВ				34.009		31.959		22.14	A
25	ATOM	1930	CG	GLU	A 31	1	32.800	30.550	31.396	1.00	26.52	A
	ATOM	1931	CD	GLU	A 31	1	31.852	31.025	32.478	1.00	31.26	A
	ATOM	1932	OE1	GLU	A 31	1	31.580	30.246	33.417	1 00	33.48	A
							31.370	32.173	32.387			
	ATOM	1933		GLU							34.81	A
	ATOM	1934	С	GLU	A 31	1	36.217	28.721	31.539	1.00	19.15	A
30	ATOM	1935	0	GLU	A 31	1	37.134	29.433	31.934	1.00	21.47	Α
	ATOM	1936	N	LYS			36.245	27.400	31.651	1 00	19.51	A
								•				-
	ATOM	1937	CA	LYS			37.394	26.749	32.258		19.17	A
	MOTA	1938	CB	LYS	A 31	5	36.946	25.514	33.043	1.00	18.84	A
	ATOM	1939	CG	LYS	A 31	5	36.280	25.885	34.368	1.00	19.62	. А
35	ATOM	1940	CD	LYS	Δ 31	5	35.653	24.696	35.073	1.00	19.22	A
55												
	MOTA	1941	CE	LYS			35.070	25.095	36.427		21.00	A
	ATOM	1942	NZ	LYS .	A 31	•	36.119	25.552	37.381	1.00	19.53	A
	ATOM	1943	С	LYS	A. 31	5	38.452	26.393	31.218	1.00	18.96	A
	ATOM	1944	ο .	LYS .	A 31	;	39.511	25.873	31.561	1 00	19.85	A
40			N	LEU			38.164	26.691			17.08	A
40	MOTA	1945							29.950			
	MOTA	1946	CA	LEU .	A 31	•	39.102	26.429	28.854	1.00	16.41	A
	ATOM	1947	CB	LEU .	A 31	5	38.414	25.636	27.738	1.00	13.81	A
	MOTA	1948	CG	LEU .	A 31	5	38.028	24.201	28.115	1.00	14.39	A
	ATOM	1949		LEU .			37.139	23.597	27.031		12.38	A
45	ATOM	1950	CD2	LEU .	A 31	•	39.302	23.373	28.309	1.00	12.77	A
	ATOM	1951	С	LEU .	A 31	5 .	39.652	27.743	28.290	1.00	17.12	A
	MOTA	1952	0	LEU .			40.851	27.860	28.023		16.53	A
		1953					38.780					
	ATOM		N	LEU .				28.729	28.105		16.27	A
	ATOM	1954	CA	LEU 2	A 31	,	39.228	30.022	27.596	1.00	17.52	A
50	ATOM	1955	CB	LEU .	A 31	,	38.083	30.752	26.887	1.00	16.37	A
	ATOM	1956	CG	LEU 2	A 31	,	37.448	29.973	25.727		18.81	A
	ATOM	1957		LEU 2			36.415	30.851	25.018		16.47	A
	MOTA	1958	CD2	LEU Z	A 31	'	38.528	29.526	24.741	1.00	17.87	A
	MOTA	1959	С	LEU Z	A 31	•	39.745	30.841	28.774	1.00	18.27	A
55	MOTA	1960	Ô	LEU Z			39.078	31.753	29.273		18.58	A
55												
	MOTA	1961	N	VAL 2			40.937	30.475	29.229		18.02	A
	ATOM	1962	CA	VAL A	A 31		41.593	31.141	30.342	1.00	18.85	A
	MOTA	1963	CB	VAL 2	A 31	:	41.846	30.153	31.500	1.00	19.91	A
	ATOM	1964		VAL 2			42.590				20.01	A
	AIOM	1904	CGI	AWP 1	- JI		44.050	30.848	32.634	1.00	20.UI	A

	ATOM	1965	CG2	VAL	Α	318		40.520.	29.584	31.990	1.00 19.44	A
•	ATOM	1966	С	VAL				42.923	31.657	29.811	1.00 19.67	A
	ATOM	1967	ō	VAL				43.690	30.902	29.208	1.00 18.26	Α
		1968	N	LEU				43.197	32.939	30.028	1.00 20.07	A
_	ATOM			LEU				44.436	33.533	29.538	1.00 20.98	A
5	ATOM	1969	CA								1.00 20.50	A
	ATOM	1970	CB	LEU				44.521	35.002	29.968		
	MOTA	1971	CG	LEU				43.418	35.908	29.408	1.00 24.38	A
	ATOM	1972		LEU				43.606	37.332	29.935	1.00 23.28	A
	MOTA ·	1973	CD2	$_{ m LEU}$	Α	319		43.453	35.887	27.875	1.00 24.33	Α
10	ATOM	1974	С	LEU	Α	319		45.680	32.774	29.994	1.00 20.38	A
	ATOM	1975	0	LEU	A	319		46.568	32.496	29.192	1.00 21.34	A
	ATOM	1976	N	ASP	Α	320		45.742	32.440	31.280	1.00 20.22	A
	ATOM	1977	CA	ASP				46.879	31.707	31.833	1.00 20.90	A
		1978	СВ	ASP			-	46.842	31.760	33.365	1.00 20.76	Α
	ATOM		CG	ASP				48.049	31.102	34.004	1.00 21.51	A
15	MOTA	1979						48.669	30.226	33.367	1.00 23.46	A
	ATOM	1980		ASP							1.00 23.89	A
	MOTA	1981		ASP				48.371	31.450	35.159		A
	MOTA	1982	С	ASP				46.814	30.247	31.367	1.00 20.06	
	MOTA	1983	0	ASP	Α	320		45.988	29.476	31.840	1.00 20.54	A
20	MOTA	1984	N	ALA:	Α	321		47.700	29.876	30.451	1.00 20.68	A
	ATOM	1985	CA	ALA	Α	321		47.733	28.522	29.903	1.00 22.04	A
	ATOM	1986	СВ	ALA				48.860	28.411	28.881	1.00 20.75	A
	ATOM	1987	C	ALA				47.858	27.400	30.940	1.00 21.62	Α.
	ATOM	1988	Ö	ALA				47.482	26.259	30.665	1.00 21.99	A,
0.5		1989	N			322.		48.372	27.715	32.127	1.00 20.89	A
25	ATOM					322		48.531	26.698	33.167	1.00 20.82	A
	ATOM	1990	CA					49.670	27.051	34.146	1.00 19.47	A
	ATOM	1991	CB			322			28.253	34.848	1.00 20.19	A
	ATOM	1992		THR				49.341		33.394	1.00 21.59	A
	ATOM	1993	CG2	THR				50.981	27.249			A
30	ATOM	1994	С			322		47.264	26.498	33.983	1.00 19.55	Ā
	ATOM	1995	0			322		47.235	25.673	34.894	1.00 21.13	
	MOTA	1996	N	LYS	Α	323.		46.216	27.248	33.661	1.00 19.33	A
	ATOM	1997	CA	LYS	Α	323		44.962	27.122	34.392	1.00 21.20	A.
	ATOM	1998	СВ			323		44.580	28.460	35.030	1.00 23.75	A
35	ATOM	1999	CG			323		45.562	28.933	36.084	1.00 28.45	A
22	ATOM	2000	CD			323		45.055	30.177	36.799	1.00 33.76	A
		2001	CE			323		46.087	30.678	37.802	1.00 36.15	Α
	ATOM		NZ			323		46.532	29.569	38.693	1.00 37.34	Α
	ATOM	2002				323		43.806	26.614	33.539	1.00 20.68	A
	ATOM	2003	C					42.649	26.757	33.915	1.00 20.42	A
40	MOTA	2004	0			323			26.019	32.392	1.00 19.97	A
•	ATOM	2005	N			324		44.114		31.531	1.00 17.98	A
	ATOM	2006	CA			324		43.060	25.494		1.00 17.50	A
	ATOM	2007	СВ			324		43.461	25.609	30.061	1.00 13.33	A
	MOTA	2008	CG			324		43.534	27.050	29.603		
45	MOTA	2009	CD	ARG	Α	324		43.996				A
	ATOM	2010	NE	ARG	Α	324		44.438	28.565	27.944	1.00 16.93	A
	MOTA	2011	CZ	ARG	Α	324		45.410	28.908	27.108	1.00 19.88	A
	ATOM	2012		ARG				46.045	27.978	26.398	1.00 14.58	Α
	ATOM	2013				324.		45.774	30.181	27.015	1.00 16.51	A
50	ATOM	2014	C			324		42.762	24.046	31.883	1.00 18.32	A
50			Ö			324		43.673	23.222	32.006	1.00 18.20	A
	MOTA	2015				325		41.479	23.748	32.055	1.00 18.32	Α
	MOTA	2016	N					41.050	22.403	32.395	1.00 17.79	`A
	ATOM	2017	CA			325		39.523	22.335	32.425	1.00 17.03	A
_	ATOM	2018	CB			325				33.116	1.00 17.03	A
55	MOTA	2019	CG			325		38.896	21.125		1.00 15.91	A
	MOTA	2020		LEU				39.392	21.048	34.557	1.00 15.93	A
	ATOM	2021	CD2	LEU				37.375	21.255	33.084		
	MOTA	2022	С			325		41.599	21.433	31.356	1.00 18.68	A
	ATOM	2023	0	LEU	JA	.325		41.347	21.586	30.157	1.00 18.28	A

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	ATOM	2024	N	GLY	А	326		42.354	20.439	31.821	1.00	18.18	. A
	ATOM	2025	CA	GLY				42.931	19.462	30.915		16.36	A
	ATOM	2026	C	GLY					19.558	30.807		19.15	A
	ATOM	2027	ō	GLY				45.093	18.592	30.404		19.52	A
5	ATOM	2028	N	CYS				45.016	20.708	31.161		18.16	A
,	ATOM	2029	CA	CYS				46.463	20.867	31.075		19.30	A
		2030	CB	CYS				46.856	22.350	31.058		20.22	A
	ATOM			CYS				46.782	23.200	32.649		21.97	A
	MOTA	2031	SG	CYS				47.169	20.157	32.228		20.22	A
10	ATOM	2032	C						19.828	33.246		17.92	A
10	ATOM	2033	0	CYS				46.561	19.020			20.51	A
	MOTA	2034	N	GLU				48.463		32.053			
	ATOM	2035	CA	GLU				49.274	19.244	33.042		23.34	A
	MOTA	2036	CB	GLU				50.710	19.139	32.507		28.68	A
	ATOM	2037	CG	GLU				50.754	18.367	31.175		38.24	
15	ATOM .	2038	CD	GLU				52.067	18.500	30.414		43.23	A
	ATOM	2039		GLU				52.535	19.643	30.218		46.22	A
	MOTA	2040	OE2	GLU				52.618	17.459	29.991		44.90	A
	MOTĄ	2041	С	GLU	Α	328		49.234	19.876	34.435		22.11	Α
	ATOM	2042	0	GLU	Α	328		49.147	19.161	35.437	1.00	20.27	A
20	ATOM	2043	N	GLU	Α	329		49.276	21.204	34.506		18.40	. A
	ATOM	2044	CA	GLU	Α	329		49.248	21.875	35.801		20.13	A
	ATOM	2045	CB	GLU	Α	329		49.587	23.363	35.657	1.00	20.36	A
•	ATOM	2046	CG	GLU	Α	329		51.014	23.651	35.190	1.00	24.05	A
	ATOM	2047	CD	GLU	Α	329		51.191	23.518	33.688	1.00	25.93	· A
25	ATOM	2048	OE1	GLU	Α	329		50.213	23.154	32.995	1.00	26.61	A
	ATOM	2049	OE2	GLU	Α	329		52.311	23.781	33.198	1.00	27.19	. A
	ATOM	2050	С	GLU	Α	329		47.890	21.718	36.480	1.00	19.36	A
	ATOM	2051		GLU				47.775	21.879	37.694	1.00	18.74	A
	ATOM	2052	N.	MET				46.863	21.415	35.691	1.00	17.28	A
30	ATOM	2053	CA	MET				45.520	21.220	36.229	1.00	16.38	A
30	ATOM	2054	СВ			330		44.474	21.833	35.294	1.00	17.65	A
	ATOM	2055	CG			330		44.460	23.365	35.311	1.00	22.95	A
		2056	SD	MET				44.186	24.026	36.979	1.00	26.78	A
	ATOM	2057	CE			330		42.435	23.712	37.186	1.00	24.69	A
35	ATOM	2058	C.	MET				45.257	19.730	36.422		14.30	A
55	ATOM	2059	o			330		44.127	19.304	36.629		15.39	A
	ATOM	2060	N .			331		46.327	18.949	36.346		15.60	A
	ATOM	2061	CA	GLU				46.289	17.501	36.531		17.08	A
	ATOM	2062	CB			331		45.607	17.155	37.862		17.00	A
40		2063	CG			331		46.070	18.027	39.038		17.46	A
40	ATOM	2063	CD			331		47.591	18.179	39.145		20.16	A
	ATOM			GLU				48.034	19.073	39.896		21.39	A
	ATOM	2065		GLU				48.345	17.420	38.500		18.87	A
	ATOM	2066						45.697	16.658	35.398		17.80	A
4.5	MOTA	2067	C			331						20.40	A
45	ATOM	2068	0			331		45.107	15.602	35.636 34.167		16.23	A
	ATOM	2069	N			332	•	45.844	17.133			14.10	A
	ATOM	2070	CA			332	•	45.420	16.353	33.015	1.00		
	ATOM	2071	C			332		43.982	16.154	32.596			A A
	ATOM	2072	0			332		43.063	16.864	33.017		11.96	
50	ATOM	2073	N			333		43.804	15.141	31.750		14.37	A
	ATOM	2074	CA			333		42.510	14.806	31.182		13.56	A
	ATOM	2075	СВ			333		42.722	13.892	29.968		15.00	A
	ATOM	2076				333		43.153	14.683	28.752		16.46	A
	MOTA	2077		TYR				42.206	15.172	27.849		15.29	A
55	ATOM	2078		TYR				42.573	16.002	26.794		13.42	A
	ATOM	2079		TYR				44.490	15.039	28.561		14.91	A
	MOTA	2080		TYR				44.872	15.877	27.499		14.87	A
	MOTA	2081	CZ			333		43.902	16.353	26.626		15.61	A
	ATOM	2082 -	ОН	TYR	A	333		44.244	17.197	25.599	1.00	17.29	A

	ATOM	2083	С	TYR	Α	333		41.470	14.230	32.127	1.00	15.23	, A
	ATOM	2084	0	TYR	А	333		40.278	14.323	31.846		16.63	Α
	ATOM	2085	N	GLY				41.907	13.650	33.244		15.50	A
		2086	CA	GLY				40.957	13.100	34.202		15.07	A
_	ATOM												
5	ATOM	2087	C	GLY				39.925	14.146	34.616		16.40	A
	MOTA	2088	0	GLY				38.724	13.946	34.433		15.05	A
	MOTA	2089	N	PRO	Α	335 .		40.366	15.278	35.184	1.00	14.96	Α
	MOTA	2090	CD	PRO	Α	335		41.727	15.531	35.689	1.00	15.88	A
	ATOM	2091	CA	PRO	A	335		39.444	16.339	35.606	1.00	15.29	A
10	ATOM	2092	CB	PRO	Α	335		40.383	17.397	36.178	1.00	13.19	A
	ATOM	2093	ĊG	PRO				41.485	16.569	36.758		13.81	А
	ATOM	2094	C	PRO				38.594	16.877	34.448		15.84	A
	ATOM	2095	Ö	PRO				37.423	17.204	34.631		14.84	A
	MOTA	2096	N	TEU				39.184	16.971	33.257		16.12	A
15	MOTA	2097	CA	LEU				38.450	17.465	32.094		15.52	A
	MOTA	2098	CB	LEU				39.396	17.653	30.898		14.39	A
	ATOM	2099	CG	LEU	Α	336		38.770	17.991	29.538	1.00	15.46	A
	MOTA	2100	CD1	LEU	Α	336		37.836	19.182	29.662	1.00	11.25	A
	MOTA	2101	CD2	LEU	Α	336		39.884	18.285	28.528	1.00	14.11	A
20	MOTA	2102	С	LEU	Α	336		37.321	16.508	31.714	1.00	16.28	A
	MOTA	2103	0	LEU				36.176	16.921	31.540	1.00	15.51	. A
	ATOM	2104	N	LYS				37.640	15.225	31.592	1.00	17.22	
	ATOM	2105	CA	LYS			•	36.624	14.243	31.235		17.39	A
							٠	37.293	12.900	30.921		17.68	A
0.5	MOTA	2106	CB	LYS						-			
25	MOTA	2107	CG	LYS				38.170	12.994	29.676		22.31	A
	ATOM	2108	CD	LYS				39.213	11.892	29.592		24.60	A
	MOTA	2109	CE	LYS				38.620	10.560	29.189		24.76	A
	MOTA	2110	NZ	LYS	Α	337		39.710	9.560	28.997		25.05	A
	ATOM	2111	С	LYS	Α	337		35.577	14.096	32.342	1.00	17.33	A
30	ATOM	2112	0	LYS	Α	337		34.456	13.652	32.090	1.00	14.42	A
	ATOM	2113	N	ALA	Α	338		35.928	14.500	33.559	1.00	15.83	A
	ATOM	2114	CA	ALA				34.989	14.395	34.674	1.00	17.52	A
	ATOM	2115	CB	ALA				35.749	14.167	35.980		19.68	A
	ATOM	2116	C	ALA				34.095	15.621	34.804		18.83	A
25		2117		ALA				33.252	15.687	35.695		18.94.	A
35	ATOM		0						16.596	33.918		19.42	A
	ATOM	2118	N	HIS				34.262					
	MOTA	2119	CA	HIS				33.438	17.796	34.004		19.28	A
	MOTA	2120	CB	HIS				33.865	18.819	32.949		19.20	A
	ATOM	2121	CG	HIS				33.163	20.134	33.074		20.26	A
40	MOTA	2122	CD2	HIS	Α	339		33.549	21.299	33.649		18.95	A
	ATOM	2123	ND1	HIS	Α	339		31.880	20.340	32.612		19.10	Α
•	ATOM	2124	CE1	HIS	Α	339		31.506	21.576	32.896		22.19	A
	ATOM	2125	NE2	HIS	Α	339		32.500	22.179	33.525	1.00	21.98	A
	ATOM	2126	С	HIS				31.957	17.448	33.845	1.00	19.13	Α
45	MOTA	2127	0	HIS				31.597	16.576	33.061	1.00	19.52	. А
	ATOM	2128	N	PRO				31.079	18.125	34.606		19.80	A
	ATOM	2129	CD	PRO				31.424	19.119	35.640		19.08	A
								29.630	17.900	34.569		20.52	A
	ATOM	2130	CA	PRO									
	MOTA	2131	CB	PRO				29.091	19.058	35.396		20.74	A
50	MOTA	2132	CG	PRO				30.146	19.207	36.454		19.20	A
	MOTA	2133	С	PRO				29.000	17.834	33.176		21.42	A
	ATOM	2134	0	PRO	Α	340		28.049	17.088	32.955		22.48	A
	ATOM	2135	N	PHE .	A	341		29.528	18.606	32.237	1.00	21.33	A
	ATOM	2136	CA	PHE .	Α	341		28.985	18.610	30.886	1.00	21.57	A
55	ATOM	2137	СВ	PHE				29.739°	19.624	30.017	1.00	21.64	Α
	ATOM	2138	CG	PHE				29.207	19.740	28.613		23.18	Α
	ATOM	2139		PHE				27.903	20.171	28.382		22.58	A
		2140		PHE		•		30.013	19.431	27.522		21.95	A
	ATOM											23.54	A
	MOTA	2141	CRI	PHE .	M	747		27.410	20.292	27.082	1.00	23.34	

									10 540	0.0.00		_
	ATOM	.2142	CE2	PHE	А	341 .		29.533	19.548	.26.220	1.00 21.83	. А
	MOTA	2143	CZ	PHE	Α	341		28.228	19.980	25.998	1.00 23.23	A
	ATOM	2144	С	PHE	Α	341		29.055	17.226	30.237	1.00 21.84	A
	ATOM	2145	ō	PHE				28.232	16.896	29.389	1.00 20.37	A
5	ATOM	2146	N	PHE				30.034	16.422	30.640	1.00 20.51	A
3							•	30.221	15.085	30.077	1.00 23.01	
	ATOM	2147	CA	PHE								A
	ATOM	2148	CB	PHE				31.710	14.809	29.850	1.00 18.00	A
	ATOM	2149	CG	PHE	Α	342		32.398	15.812	28.971	1.00 17.05	A
	ATOM	2150	CD1	PHE	Α	342		32.010	15.987	27.652	1.00 17.78	Α
10	ATOM	2151	CD2	PHE	Α	342		33.487	16.534	29.450	1.00 15.72	A
	ATOM	2152		PHE				32.702	16.867	26.811	1.00 18.08	Α
	ATOM	2153		PHE				34.184	17.414	28.617	1.00 17.45	A
	ATOM	2154	CZ	PHE				33.790	17.578	27.298	1.00 16.56	A
				PHE				29.679	13.972	30.976	1.00 24.95	A
	ATOM	2155	C				•					
15	MOTA	2156	0	PHE				30.002	12.798	30.777	1,00 23.95	A
	MOTA	2157	N	GLU	A	343		28.861	14.333	31.958	1.00 27.35	A
	ATOM	2158	CA	GLU	Α	343		28.325	13.349	32.897	1.00 30.28	A
	ATOM	2159	CB	GLU	Α	343		27.187	13.964	33.716	1.00 32.20	A
	ATOM	2160	CG	GLU	Α	343		26.581	12.991	34.714	1.00 39.71	Α
20	ATOM	2161	CD	GLU	Α	343		25.628	13.661	35.688	1.00 44.72	A
20	MOTA	2162		GLU				24.661	14.314	35.234	1.00 47.55	А
		2163		GLU				25.847	13.526	36.911	1.00 46.89	A
	ATOM			GLU				27.852	12.017	32.305	1.00 28.98	A
	ATOM	2164	С							32.800	1.00 20.30	A
	MOTA	2165	0	GLU				28.225	10.952			
25	MOTA	2166	N	SER				27.037	12.067	31.258	1.00 26.09	A
	MOTA	2167	CA	SER	Α	344		26.520	10.838	30.656	1.00 28.36	A
	ATOM	2168	CB	SER	Α	344		25.129	11.089	30.067	1.00 28.73	A
	MOTA	2169	OG	SER	Α	344		25.203	11.942	28.940	1.00 30.91	A
	MOTA	2170	С	SER	Α	344		27.407	10.214	29.577	1.00 27.66	Α
30	ATOM	2171	0	SER				26.987	9.281	28.900	1.00.28.66	A
30	ATOM	2172	N	VAL				28.627	10.715	29.419	1.00 26.75	A
		2173	CA	VAL				29.534	10.183	28.402	1.00 23.44	A
	MOTA							30.565	11.256	27.950	1.00 23.10	A
	ATOM	2174	CB	VAL				31.589	10.631	26.995	1.00 22.24	A
	ATOM	2175		VAL								A
35	ATOM	2176		VAL				29.854	12.418	27.275	1.00 20.05	
	MOTA	2177	С	VAL				30.326	8.957	28.855	1.00 24.26	A
	MOTA	2178	0	VAL	А	345		30.876	8.930	29.960	1.00 22.83	A
	ATOM	2179	N	THR	Α	346		30.374	7.942	27.997	1.00 21.77	A
	ATOM	2180	CA	THR	Α	346		31.153	6.740	28.272	1.00 23.70	A
40	ATOM	2181	CB	THR	Α	346		30.391	5.455	27.857	1.00 26.53	A
	ATOM	2182		THR				29.248	5.284	28.706	1.00 29.98	A
	ATOM	2183		THR				31.289	4.231	27.990	1.00 24.28	А
		2184	C	THR				32.383	6.945	27.385	1.00 23.43	A
	ATOM							32.305	6.827	26.160	1.00 24.50	
	MOTA	2185	0	THR	_							
45	MOTA	2186	И	TRP				33.508	7.270		1.00 22.98	
	ATOM	2187	CA	TRP				34.744	7.569	27.300	1.00 23.81	A
	MOTA	2188	CB	TRP	Α	347		35.683	8.352	28.219	1.00 22.54	A
	ATOM	2189	CG	TRP	Α	347		35.128	9.658	28.693	1.00 20.61	A
	ATOM	2190	CD2	TRP	A	347		35.257	10.927	28.040	1.00 19.11	A
50	ATOM	2191		TRP				34.581	11.881	28.838	1.00 18.39	A
	ATOM	2192		TRP				35.878	11.351	26.858	1.00 18.16	Α
•	ATOM	2193		TRP				34.397	9.883	29.828	1.00 18.35	A
								34.065	11.218	29.923	1.00 19.51	A
	ATOM	2194		TRP							1.00 16.88	A
	ATOM	2195		TRP				34.510	13.234	28.491		
55	ATOM	2196		TRP				35.808	12.701	26.511	1.00 17.23	A
	MOTA	2197		TRP				35.127	13.624	27.327	1.00 18.16	A
	ATOM	2198	C	TRP				35.538	6.429	26.675	1.00 25.79	A
	ATOM	2199	0	TRP				36.304	6.654	25.742	1.00 24.67	A
	MOTA	2200	N	ALA	A	348		35.360	5.215	27.183	1.00 27.10	A

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	ATOM .	2201	CA	ALA A	348	36.116	4.063	26.697	1.00 27.46	A
	ATOM	2202	СВ	ALA A	348	35.899	2.869	27.636	1.00 27.09	A
	ATOM	2203	С	ALA A	348	35.895	3.620	25.256	1.00 27.18	A
	MOTA	2204	0	ALA A	348	36.830	3.148	24.613	1.00 29.41	A
5	ATOM	2205	N	ASN A	349	34.682	3.769	24.735	1.00 26.55	A
	ATOM	2206	CA	ASN A	349	34.418	3.310	23.375	1.00 27.28	A
	ATOM	2207	CB	ASN A	349	33.700	1.962	23.444	1.00 29.37	A
	MÖTA	2208	CG	ASN A	349	32.299	2.088	24.013	1.00 30.92	A
	MOTA	2209	OD1	ASN A		32.045	2.942	24.859	1.00 30.17	A
10	ATOM	2210	ND2	ASN A	349	31.386	1.237	23.553	1.00 33.52	A
	ATOM	2211	C .	ASN A	349	33.599	4.265	22.509	1.00 26.47	A
	ATOM	2212	0	ASN A		32.669	~ 3.843	21.819	1.00 25.87	Α
	ATOM	2213	N	LEU A	350	33.947	5.543	22.518	1.00 24.45	A
	MOTA	2214	CA	LEU A	350	33.203	6.510	21.721	1.00 23.14	A
15	ATOM	2215	CB	LEU A	350	33.837	7.898	21.848	1.00 23.22	A
	ATOM	2216	CG	LEU A	350	33.659	8.605	23.191	1.00 21.05	A
	ATOM	2217	CD1	LEU A	350	34.646	⁻ 9.756	23.293	1.00 19.36	A
	ATOM	2218	CD2	LEU A	350	32.220	9.094	23.319	1.00 18.78	A
	ATOM	2219	С	LEU A	350	33.082	6.152	20.240	1.00 22.60	A
20	ATOM	2220	0	LEU A	350	32.011	6.296	19.650	1.00 21.15	A
	ATOM	2221	N	HIS A	351	34.165	5.689	19.627	1.00 23.13	A
	ATOM	2222	CA	HIS A	351	34.089	5.387	18.204	1.00 27.83	A
	ATOM	2223	CB	HIS A	351	35.506	5.325	17.596	1.00 29.36	A
	ATOM	2224	CG	HIS A	351	36.082	3.950	17.493	1.00 32.07	A
25	ATOM	2225	CD2	HIS A	351	36.611	3.128	18.431	1.00 32.39	A
	ATOM	2226	NĎ1	HIS A	351	36.197	3.285	16.291	1.00 33.02	A
	ATOM	2227	CE1	HIS A	351	36.775	2.113	16.493	1.00 33.58	. A
	ATOM	2228	NE2	HIS A	351	37.036	1.992	17,782	1.00 31.76	A
	ATOM	2229	С	HIS A	351	33.258	4.144	17.874	1.00 28.12	A
30	ATOM	2230	0	HIS A	351	33.015	3.847	16.707	1.00 29.49	A
	ATOM	2231	N	GLN A	352	32.800	3.442	18.908	1.00 29.28	A
	ATOM	2232	CA	GLN A	352	31.963	2.255	18.726	1.00 29.67	A
	ATOM	2233	CB	GLN A	352	32.366	1.145	19.694	1.00 30.56	A
	ATOM	2234	CG	GLN A		33.169	0.041	19.041	1.00 30.88	A
35	ATOM	2235	CD	GLN A		34.493	-0.186	19.729	1.00 31.21	A
	ATOM	2236	OEl				-0.450	20.928	1.00 30.76	A
	ATOM	2237	NE2			35.578	-0.084	18.971	1.00 32.30	A
	ATOM	2238	C	GLN A		30.504	2.638	18.963	1.00 30.42	A.
	ATOM	2239	0	GLN A		29.595	1.831	18.770	1.00 29.01	A
40	ATOM	2240	N	GLN A		30.290	3.875	19.397	1.00 27.64	A
	MOTA	2241	CA	GLN A		28.948	4.365	19.652	1.00 27.42	A
	ATOM	2242	CB	GLN A		28.977	5.401	20.775	1.00 25.77	A
	ATOM	2243	CG	GLN A		29.408	4.837	22.115	1.00 27.34	A
	ATOM	2244	CD	GLN A		29.638	5.914	23.156	1.00 27.19	
45	ATOM	2245		GLN A		28.875	6.872	23.252	1.00 28.29	
	ATOM	2246		GLN A		30.687	5.753	23.951	1.00 28.79	A
	ATOM	2247	С	GLN A		28.375	4.989	18.385	1.00 29.00	A
	ATOM	2248	0	GLN A		29.118	5.455	17.516	1.00 29.14	A
	ATOM	2249	N	THR A		27.053	4.984	18.276	1.00 27.31	A
50	MOTA	2250	CA	THR A		26.390	5.568	17.119	1.00 27.85	A A
	ATOM	2251	CB	THR A		24.991	4.941	16.904	1.00 30.69	A
	ATOM	2252		THR A		25.132	3.532	16.665	1.00 30.07	A
	ATOM	2253	CG2			24.289	5.585	15.709	1.00 29.58	A
	ATOM	2254	C	THR A		26.244	7.062	17.376	1:00 26.85 1.00 25.77	A
55	ATOM	2255	0	THR A		25.592	7.475	18.329	1.00 25.77	A
	ATOM	2256	N	PRO A		26.867	7.898	16.533 15.431	1.00 27.22	A
	ATOM	2257	CD	PRO A		27.792	7.588		1.00 25.89	A
	ATOM	2258	CA	PRO A		26.763	9.346	16.734	1.00 27.23	A
	ATOM	2259	CB	PRO A	222	27.625	9.915	15.609	T.OO .C#.31	n

	ATOM	2260	CG	PRO A		28.643	8.838	15.385	1.00 25.54		A
	ATOM	2261	C	PRO A	355	25.322	9.837	16.641	1.00 28.07		Α
	AŢOM	2262	0	PRO A	355	24.548	9.364	15.810	1.00 27.24		A
	ATOM	2263	N	PRO A	356	24.941	10.792		1.00 28.28		A
5	ATOM	2264	CD	PRO A	356	25.752	11.560		1.00 28.31		A
	ATOM	2265	CA	PRO A	356	23.572	11.306		1.00 28.44		A
	ATOM	2266	CB	PRO A		23.539	12.301		1.00 28.11		A
	ATOM	2267	CG	PRO A		24.946	12.832		1.00 26.86		A
	ATOM	2268	C	PRO A		23.363	11.978	16.097	1.00 29.25		A
10	ATOM	2269	ō	PRO A		24.304	12.537	15.529	1.00 27.27		A
10	ATOM	2270	N	ALA A		22.143	11.910	15.575	1.00 27.27		
	ATOM	22.71	CA	ALA A		21.848	12.521				A
	ATOM	2272	CB	ALA A		20.507	12.019	14.287	1.00 32.81		A
			CD	ALA A				13.757	1.00 31.99		A
15	MOTA	2273				21.824	14.035	14.448	1.00 35.05		A
15	ATOM	2274	0	ALA A		21.194	14.561	15.369	1.00 35.04		A
	ATOM	2275	N	LEU A		22.516	14.730	13.552	1.00 37.81		Α
	ATOM	2276	CA	LEU A		22.578	16.185	13.597	1.00 42.15		Α
	ATOM	2277	CB	LEU A		23.679	16.681	12.658	1.00 39.54		A
	MOTA	2278	CG	LEU A		25.086	16.285	13.109	1.00 39.51		Α
20	MOTA	2279		LEU A		26.102	16.686	12.062	1.00 39.29		Α
	MOTA	2280	CD2	LEU A		25.395	16.953	14.445	1.00 40.01		Α
	ATOM	2281	C	LEU A	358	21.241	16.837	13.242	1.00 45.91		Α
	ATOM	2282	0	LEU A	358	20.874	16.927	12.069	1.00 45.71		A
	MOTA	2283	N	THR A	359	20.530	17.290	14.275	1.00 50.06		Α
25	ATOM	2284	CA	THR A	359	19.223	17.939	14.140	1.00 53.73		Α
	ATOM	2285	CB	THR A	359	19.353	19.428	13.726	1.00 54.04	٠	Α
	ATOM	2286	OG1	THR A	359	19.995	19:521	12.448	1.00 56.35		Α
	ATOM	2287	CG2	THR A	359	20.158	20.204	14.763	1.00 54.32		Α
	ATOM	2288	С	THR A	359	18.309	17.236	13.139	1.00 54.47		Α
30	ATOM	2289	0	THR A		18.483	16.016	12.930	1.00 55.90		A
	ATOM	2290	OXT			17.407	17.908	12.595	1.00 56.97		A
	TER										
	ATOM	1	CB	PRO B	71	99.838	54.646	-7.659	1.00 20.00	6	
	ATOM	2	CG	PRO B	71	99.216	55.105	-6.341	1.00 20.00	6	
35	MOTA	3	С	PRO B	71	98.903	54.776	-9.981	1.00 20.00	6	
	ATOM	4	0	PRO B	71	98.022		-10.109	1.00 20.00	8	
	ATOM	5	N	PRO B	71	97.782	55.851	-8.042	1.00 20.00	7	
	ATOM	6	CD	PRO B	.71	97.728	55.323	-6.668	1.00 20.00	6	
	ATOM	7	CA	PRO B	71	99.087	55.515	-8.658	1.00 20.00	6	
40	ATOM	8	N	PRO B	72	99.732		-10.985	1.00 20.00	7	
	ATOM	9	CD	PRO B	72	100.794		-10.977	1.00 20.00	6	
	ATOM	10	CA	PRO B	72	99.645		-12.297	1.00 20.00	6	
	ATOM	11	CB	PRO B	72	100.885		-13.017	1.00 20.00	6	
	ATOM	12	CG	PRO B	72	100.003		-12.456			
45			_						1.00 20.00	6	
73	ATOM ATOM	13	C	PRO B	72	99.627		-12.202	1.00 20.00	6	
		14	0	PRO B	72	100.246		-11.314	1.00 20.00	8	
	ATOM	15	N	ALA B	73	98.906		-13.122	1.00 20.00	7	
	MOTA	16	CA	ALA B	73	98.805		-13.167	1.00 20.00	6	
50	ATOM	17	CB	ALA B	73	97.420		-12.710	1.00 20.00	6	
50	ATOM	18	С	ALA B	73	99.053		-14.604	1.00 20.00	6	
	ATOM	19	0	ALA B	73	99.027		-15.526	1.00 20.00	8	
	ATOM	20	N	PRO B	74	99.313		-14.818	1.00 20.00	7	
	MOTA	21	CD	PRO B	74	99.473		-13.857	1.00 20.00	6	
	ATOM	22	CA	PRO B	74	99.553		-16.189	1.00 20.00	6	
55	ATOM	23	CB	PRO B	74	99.700.		-16.023	1.00 20.00	6	
	ATOM	24	CG	PRO B	74	100.292	47.004	-14.649	1.00 20.00	6	
	ATOM	25	С	PRO B	74	98.371	49.018	-17.079	1.00 20.00	6	
	ATOM	26	0	PRO B	74	97.279	49.296	-16.583	1.00 20.00	8	
	ATOM	27	N	ALA B	75	98.589			1.00 20.00	7	

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	ATOM	28	CA	ALA.	В	75	97.516	49.368	-19.321	1.00	20.00	6
	ATOM	29	CB	ALA	В	75	98.061	49.462	-20.745	1.00	20.00	6
	ATOM	30	С	ALA	В	75	96.446	48.285	-19.246	1.00	20.00	6
	ATOM	31	0	ALA	В	75	96.745	47.126	-18.961	1.00	20.00	8
5	ATOM	32	N	LYS	В	76	95.200	48.666	-19.494	1.00	20.00	7
_	ATOM	33	CA	LYS		76	94.098	47.716	-19.463.		20.00	6
	ATOM	34	СВ	LYS		76	92.793		-19.805		20.00	6
	ATOM	35	CG	LYS		76	91.546	-	-19.225		20.00	6
	ATOM	36	CD	LYS		76	91.511		-17.711		20.00	6
10	ATOM	37	CE	LYS	_	76 ·	90.184		-17.152		20.00	6
10	ATOM	38	NZ	LYS		76	90.108		-15.673		20.00	7
		39	C	LYS		76 .	94.389	•	-20.513		20.00	6
	ATOM	40		LYS		76 . 76	94.736		-21.645		20.00	8
	ATOM		0			70 77	94.750		-20.145		20.00	7
15	ATOM	41	N	LYS					-21.107			6
15	ATOM	42	CA	LYS		77	94.525				20.00	
	ATOM	43	CB	LYS		77	94.875		-20.384		20.00	6
	ATOM	44	CG	LYS		77	96.117		-19.506		20.00	6
	ATOM	45	CD	LYS		77 .	96.461		-18.842		20.00	6
	MOTA	46	CE	LYS		77	97.501		-17.745		20.00	6
20	ATOM	47	NZ	LYS		77	98.771		-18.255		20.00	7
	ATOM	48	С	LYS		77	93.311		-22.012		20.00	6
	ATOM	49	0	LYS		77	92.218		-21.704		20.00	8
	ATOM	50	N	ARG		78	93.514		-23.129		20.00	7
	ATOM	51·	CA	ARG		78 ·	92.442		-24.086		20.00	6
25	ATOM	52	CB	ARG		78	92.465		-25.193		20.00	6
	ATOM	53	CG	ARG		78	93.787		-25.925		20.00	6
	ATOM	54	CD	ARG	В	78	93.833		-26.771		20.00	6
	ATOM	55	NE	ARG		78	95.052		-27.575		20.00	7
	MOTA	56	CZ	ARG		78	96.287		-27.078		20.00	6
30	ATOM	57	NH1	ARG	В	78	96.486	45.721	-25.764	1.00	20.00	7
	ATOM	58	NH2	ARG	В	78	97.330		-27.897	1.00	20.00	7
	ATOM	59	С	ARG	В	78	92.570		-24.678	1.00	20.00	6
	ATOM	60	0	ARG	В	78	93.625	41.126	-24.581	1.00	20.00	8
	ATOM	61	N	PRO	В	79	91.494	41.240	-25.303	1.00	20.00	7
35	ATOM	62	CD	PRO	В	79	90.195	-41.894	-25.543	1.00	20.00	6
	ATOM	63	CA	PRO	В	79	91.519	39.899	-25.896	1.00	20.00	6
	ATOM	64	CB	PRO	в	79	90.214	39.848	-26.691	1.00	20.00	6
	ATOM	65	CG	PRO	В	79	89:304	40.725	-25.889	1.00	20.00	6
	ATOM	66	. C	PRO	В	79	92.737	39.614	-26.778	1.00	20.00	6
40	ATOM	67	0	PRO	В	79	93.311	38.523	-26.717	1.00	20.00	8
	ATOM	68	N	GLU	В	80	93.124	40.597	-27.589	1.00	20.00	7
	ATOM	69	·CA	GLU	в	80	94.254	40.441	-28.503	1.00	20.00	6
	ATOM	70	СВ	GLU	В	80	94.358	41.644	-29.446	1.00	20.00	6
	ATOM	71	CG	GLU	В	80	94.881	42.912	-28.800	1.00	20.00	6
45	ATOM	72	CD	GLU	В	80	95.009		-29.788	1.00	20.00	6
	ATOM	73		GLU		80	93.968		-30.308		20.00	8
	ATOM	74		GLU		80	96.150		-30.047		20.00	8
	ATOM	75	С	GLU		80	95.591		-27.787	1.00	20.00	6.
	ATOM	76	ō	GLU		80	96.558		-28.405	1.00	20.00	8
50	ATOM	77	N	ASP		81	95.656		-26.497		20.00	7
	ATOM	78	CA	ASP		81	96.902		-25.749		20.00	6
	ATOM	79	СВ	ASP		81	96.888		-24.446		20.00	6
	ATOM ·	80	CG	ASP		81	96.774		-24.682		20.00	6
	ATOM	81		ASP		81	97.436		-25.606		20.00	8
55	ATOM	82		ASP		81	96.033		-23.933		20.00	8
55	ATOM	83	C	ASP		81	97.111		-25.393		20.00	6
	ATOM	84	ō	ASP		81	98.172		-24.890		20.00	8
	ATOM	85	N	PHE		B2	96.103		-25.679		20.00	7
		86	CA	PHE		82 82	96.140		-25.340		20.00	6
	ATOM	00	CM	EIIE .	، ب	. .	20. TAO	50.077	20.040	4.00	50.00	9

	MOTA	87	CB	PHE	·B	82			36.369 -24.302 1.00 20.00 6
	MOTA	88	CG	PHE		82		95.157	37.187 -23.050 1.00 20.00 6
	ATOM	89	CD1	PHE	В	82		95.880	36.724 -21.959 1.00 20.00 6
	MOTA	90	CD2	PHE	В	82		94.525	38.423 -22.961 1.00 20.00 6
5	ATOM	91	CEl	PHE	В	82		95.976	37.479 -20.793 1.00 20.00 6
	ATOM	92	CE2	PHE	В	82		94.615	39.188 -21.800 1.00 20.00 6
	ATOM	93	CZ	PHE		82		95.343	38.712 -20.713 1.00 20.00 6
	ATOM	94	C	PHE		82		95.929	35.719 -26.496 1.00 20.00 6
	ATOM	95	ō	PHE		82		95.342	36.061 -27.524 1.00 20.00 8
10	ATOM	96	N	LYS		83		96.406	34.500 -26.286 1.00 20.00 7
10	ATOM	97	CA	LYS		83		96.242	33.411 -27.228 1.00 20.00 6
	MOTA	98	CB	LYS		83		97.594	32.777 -27.562 1.00 20.00 6
	ATOM	99	CG	LYS		83		97.503	31.531 -28.425 1.00 20.00 6
		100	CD	LYS		83		98.888	31.074 -28.856 1.00 20.00 6
1.5	ATOM		CE	LYS				98.826	29.808 -29.699 1.00 20.00 6
15	ATOM	101				83			
	MOTA	102		LYS		83		98.287	
	ATOM	103	C	LYS		83		95.387	
•	ATOM	104	0	LYS		83		95.884	
	ATOM	105	N	PHE		84		94.094	32.393 -26.710 1.00 20.00 7
20	ATOM	106	CA	PHE		84		93.217	31.511 -25.958 1.00 20.00 6
	MOTA	107	CB	PHE		84		91.758	31.928 -26.133 1.00 20.00 6
	MOTA	108	CG	PHE		84		91.426	33.228 -25.462 1.00 20.00 6
	ATOM	109		PHE		84		91.668	34.439 -26.099 1.00 20.00 6
	MOTA	110		PHE		84		90.907	33.243 -24.174 1.00 20.00 6
25	MOTA	111		PHE		84		91.400	35.644 -25.464 1.00 20.00 6
	MOTA	112	CE2	PHE	В	84		90.636	34.447 -23.528 1.00 20.00 6
	MOTA	113	CZ	PHE		84		90.884	35.646 -24.176 1.00 20.00 6
	ATOM	114	С	PHE		84		93.402	30.054 -26.335 1.00 20.00 6
	MOTA	115	0	PHE		84		93.734	29.734 -27.476 1.00 20.00 8
30	MOTA	116	N	GLY	В	85		93.196	29.178 -25.359 1.00 20.00 7
	ATOM	117	CA	GLY	В	85		93.349	27.758 -25.591 1.00 20.00 6
	MOTA	118	С	GLY	В	85		92.103	26.977 -25.221 1.00 20.00 6
	ATOM	119	Ο.	GLY	В	85		90.982	27.393 -25.525 1.00 20.00 8
	MOTA	120	N	LYS	В	86		92.296	25.858 -24.534 1.00 20.00 7
35	MOTA	121	CA	LYS	В	86		91.182	25.005 -24.153 1.00 20.00 6
	MOTA	122	CB	LYS	В	86		91.695	23.640 -23.687 1.00 20.00 6
	MOTA	123	CG	LYS	В	86		92.421	23.667 -22.356 1.00 20.00 6
	MOTA	124	CD	LYS	В	86		92.855	22.272 -21.941 1.00 20.00 6
	ATOM	125	CE	LYS	В	86		93.685	22.319 -20.668 1.00 20.00 6
40	ATOM	126	NZ	LYS	В	86		94.209	20.975 -20.287 1.00 20.00 7
	ATOM	127	С	LYS	В	86		90.267	25.576 -23.077 1.00 20.00 6
	MOTA	128	0	LYS	В	86		90.668	26.410 -22.260 1.00 20.00 8
	ATOM	129	N	ILE	В	87		89.026	25.106 -23.102 1.00 20.00 7
	ATOM	130	CA	ILE	В	87		88.023	25.497 -22.131 1.00 20.00 6
45	MOTA	131	CB	ILE	В	87		86.604	25.159 -22.647 1.00 20.00 6
	ATOM	132		ILE		87		85.582	25.261 -21.503 1.00 20.00 6
	MOTA	133		ILE		87		86.260	26.085 -23.820 1.00 20.00 6
	ATOM	134		ILE		87		84.912	25.819 -24.463 1.00 20.00 6
	ATOM	135	С	ILE		87		88.312	24.687 -20.872 1.00 20.00 6
50	ATOM	136	Ō	ILE		87		88.396	23.461 -20.927 1.00 20.00 8
	ATOM	137	N·	LEU		88		88.473	25.368 -19.742 1.00 20.00 7
	ATOM	138	CA	LEU		88	•	88.757	24.686 -18.486 1.00 20.00 6
	ATOM	139	СВ	LEU		88		89.592	25.586 -17.575 1.00 20.00 6
	ATOM	140	CG	LEU		88		90.968	25.987 -18.112 1.00 20.00 6
55	ATOM	141		LEU		88		91.611	27.006 -17.186 1.00 20.00 6
23	ATOM	142		LEU		88		91.836	24.756 -18.234 1.00 20.00 6
	ATOM	143	C	LEU		88		87.471	24.298 -17.776 1.00 20.00 6
	ATOM .	144	0	LEU		88		87.434	23.334 -17.014 1.00 20.00 8
		145	N	GLY		89		86.410	25.051 -18.024 1.00 20.00 7
	ATOM	747	TA	יניני	יב	0)		00.310	20.001 20.021 2.00 20.00 /

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ATOM
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     ATOM
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20
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    ATOM
             188
                              95
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    ATOM
             189
                  CG2 THR B
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             198
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                  CG1 VAL B
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    MOTA
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                  CG2 VAL B
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    MOTA
             204
                  C
                       VAL B
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	ATOM	205	0	VAL	В	97	91.122	30.698 -19.889	1.00 20.00	8
•	ATOM	206	N .	LEU	В	98	91.617	28.690 -20.770	1.00 20.00	7
	ATOM	207	CA	LEU	В	98	93.039	28.821 -20.499	1.00 20.00	6
	ATOM	208	CB	LEU	В	98	93.727	27.459 -20.618	1.00 20.00	6
5	ATOM	209	CG	LEU	В	98	95.240	27.421 -20.383	1.00 20.00	6
_	ATOM	210	CD1	LEU	В	98	95.565	28.019 -19.021	1.00 20.00	. 6
	ATOM	211	CD2	LEU	В	98	95.739	25.987 -20.463	1.00 20.00	6
	ATOM	212	С	LEU	В	98	93.580	29.785 -21.552	1.00 20.00	6
	ATOM	213	0	LEU	В	98	93.293	29.637 -22.738	1.00 20.00	8
10	ATOM	214	N	ALA	В	99	94.343	30.783 -21.121	1.00 20.00	7
	ATOM	215	CA	ALA		99	94.897	31.767 -22.043	1.00 20.00	6
	ATOM	216	СВ	ALA		99	94.087	33.055 -21.980	1.00 20.00	6
	ATOM	217	С	ALA	В	99	96.353	32.067 -21.723	1.00 20.00	6
	ATOM	218	0	ALA		99	96.748	32.110 -20.554	1.00 20.00	8
15	ATOM	219	N	ARG	В	100	97.152	32.270 -22.763	1.00 20.00	7
	ATOM	220	CA	ARG			98.554	32.596 -22.568	1.00 20.00	6
	ATOM	221	СВ	ARG			99.442	31.657 -23.393	1.00 20.00	6
	ATOM	222	CG	ARG			100.934	31.833 -23.131	1.00 20.00	6
	ATOM	223	CD	ARG	В	100	101.770	30.835 -23.923	1.00 20.00	6
20	ATOM	224	NE	ARG	В	100	101.600	29.452 -23.469	1.00 20.00	7
	ATOM	225	CZ	ARG	в	100	102.059	28.970 -22.314	1.00 20.00	6
	ATOM	226	NH1	ARG	В	100	102.722	29.752 -21.473	1.00 20.00	7
	ATOM	227	NH2	ARG	В	100	101.864	27.694 -22.003	1.00 20.00	7
	ATOM	228	C	ARG	В	100	98.756	34.045 -23.004	1.00 20.00	6
25	MOTA	229	0	ARG	В	100	98.454	34.408 -24.146	1.00 20.00	8
	ATOM	230	N	GLU	В	101	99.228	34.883 -22.087	1.00 20.00	7
	MOTA	231	CA	GLU	В	101	99.470	36.286 -22.408	1.00 20.00	6
	ATOM	232	CB	GLU	В	101	99.709	37.091 -21.123	1.00 20.00	6
	ATOM	233	CG	GLU	В	101	99.986	38.571 -21.363	1.00 20.00	6
30	MOTA	234	CD	GLU	В	101	100.164	39.347 -20.075	1.00 20.00	6
	ATOM	235	OE1	GLU	В	101	100.717	38.780 -19.114	1.00 20.00	8
	ATOM	236	OE2	GLU	В	101	99.765	40.531 -20.025	1.00 20.00	8
	MOTA	237	С	GLU			100.703	36.338 -23.317	1.00 20.00	6
	ATOM	238	Ο _	GLU			101.773	35.865 -22.944	1.00 20.00	8
35	MOTA	239	N	LEU			100.546	36.909 -24.507	1.00 20.00	7
	ATOM	240	CA	LEU.			101.632	36.982 -25.482	1.00 20.00	6
	MOTA	241	СВ	LEU			101.145	37.683 -26.753	1.00 20.00	6
	MOTA	242	CG	LEU			100.013	36.985 -27.517	1.00 20.00	6
	ATOM	243		LEU			99.500	37.897 -28.623	1.00 20.00	6
40	MOTA	244		LEU			100.517	35.670 -28.089	1.00 20.00	6
	ATOM	245	С	LEU			102.906	37.663 -25.000	1.00 20.00	6
	ATOM	246	0	LEU			104.000	37.137 -25.180	1.00 20.00	8
	ATOM	247	N	ALA			102.760	38.828 -24.382	1.00 20.00 1.00 20.00	7 6
45	ATOM	248	CA	ALA			103.909	39.587 -23.910	1.00 20.00	6
45	ATOM	249	СВ	ALA			103.464	41.002 -23.546	1.00 20.00	
	ATOM	250	С	ALA			104.697	38.983 -22.747		6
	ATOM	251	0	ALA			105.832	39.389 -22.503 38.007 -22.050	1.00 20.00 1.00 20.00	8 7
	ATOM	252	N	THR			104.122 104.790	37.418 -20.893	1.00 20.00	6
50 .	ATOM	253	CA	THR				37.799 -19.592	1.00 20.00	6
50	ATOM	254	CB	THR			104.059 102.712	37.303 ~19.648	1.00 20.00	8
	ATOM	255		THR				39.313 -19.404	1.00 20.00	6
	ATOM	256 257		THR			104.033 104.880	35.902 -20.901	1.00 20.00	6
	ATOM	257 258	С 0	THR			104.680	35.323 -20.160	1.00 20.00	8
55	ATOM ATOM	259	N	SER			104.042	35.274 -21.722	1.00 20.00	7
23	ATOM	260	CA	SER			103.950	33.818 -21.842	1.00 20.00	6
	ATOM	261	CB	SER			105.344	33.213 -22.048	1.00 20.00	6
	ATOM	262	OG	SER			105.264	31.819 -22.287	1.00 20.00	8
	ATOM	263	C.	SER			103.204	33.243 -20.576	1.00 20.00	6
	ALON	200		711	ب		200.003	23.213 20.070		٠.

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	ATOM	264	<u>o</u>	SER	В	105	103.286	32.029	-20.363	1.00	20.00	8	
	ATOM	265	N	ARG	В	106	102.771	34.124	-19.736	1.00	20.00	7	
	ATOM	266	CA	ARG	В	106	102.089		-18.509	1.00	20.00	6	
	ATOM	267	CB	ARG	В	106	101.833	34.914	-17.598	1.00	20.00	6	
5	MOTA	268	CG	ARG			103.022		-16.781		20.00	6	
	ATOM	269	CD	ARG	В	106	102.724	36.653	-16.045		20.00	6	
	ATOM	270	NE	ARG	В	106	103.756	36.940	-15.051	1.00	20.00	7	
	ATOM	271	CZ	ARG			103.964		-14.504		20.00	6	
	ATOM	272		ARG			103.210		-14.858		20.00	7	
10	ATOM	273	NH2	ARG			104.918		-13.590		20.00	. 7	
	ATOM	274	С	ARG			100.743		-18.856		20.00	6	
	ATOM	275	0	ARG			100.069		-19.777		20.00	8	
	ATOM	276	N	GLU			100.354		-18.115		20.00	7	
	ATOM	277	CA	GLU			99.072		-18.336		20.00	6	
15	ATOM	278	CB	GLU			99.193		-18.212		20.00	6	
	ATOM	279	CG.	GLU			100.180		-19.144		20.00	6	
	ATOM	280	CD	GLU			100.124		-19.023		20.00	6	
	ATOM	281		GLU			99.373		-19.798		20.00	. 8	
	ATOM	282	OE2				100.813		-18.138		20.00	8	
20	ATOM	283	С	GLU			98.070		-17.285		20.00	6	
	ATOM	284	0	GLU			98.368		-16.095		20.00	8 7	
	ATOM	285	N	TYR			96.885		-17.727		20.00	6	
	ATOM	286	CA	TYR			95.829		-16.817		20.00	6	
	ATOM	287	CB	TYR			95.525		-16.979		20.00	6	
25	ATOM	288	CG	TYR			96.603 96.744		-16.487 -15.129		20.00	6	
	ATOM	289	CD1	TYR TYR			97.727		-14.674		20.00	6	
	ATOM	290					97.467		-17.386		20.00	6	
	ATOM	291	CD2 CE2				98.442		-16.950		20.00	6	
20	ATOM	292 293	CZ	TYR			98.569		-15.599		20.00	6	
30	ATOM ATOM	294	OH	TYR			99.529		-15.187		20.00	8	
	ATOM	295	C	TYR			94.566		-17.167		20.00	6	
	ATOM	296	Ö	TYR			94.389		-18.306		20.00	8	
	ATOM	297	N	ALA			93.697		-16.181		20.00	7	
35	ATOM	298	CA			109	92.421		-16.414	1.00	20.00	6.	
55	ATOM	299	CB	ALA			92.024		-15.214		20.00	6	
	ATOM	300	C	ALA			91.513	32.288	-16.542	1.00	20.00	6	
	ATOM	301	0	ALA			91.278	33.003	-15.558	1.00	20.00	8	
	ATOM	302	N			110	91.042	32.557	-17.756		20.00	7	
40	MOTA	303	CA	ILE	В	110	90.186	33.711	-17.968	1.00	20.00	6	
	ATOM.	304	CB	ILE	В	110	90.574		-19.271	1.00	20.00	6	
	ATOM	305	CG2	ILE	В	110	89.628		-19.507	1.00	20.00	6	
	MOTA	306	CG1	ILE	В	110	92.023		-19.159		20.00	6	
	MOTA	307	CD1	ILE			92.487		-20.312		20.00	6	
45	MOTA	308	С			110	88.715		-18.004		20.00	6	
	MOTA	309	0			110	88.285		-18.851		20.00	8	
	MOTA	310	N	LYS			87.956		-17.052		20.00	7	
	MOTA	311	CA	LYS			86.527		-16.975		20.00	6	
	MOTA	312	CB	LYS			86.022		-15.531		20.00	6	
50	ATOM	313	CG	LYS			84.509		-15.411		20.00	6	
	MOTA	314	CD	LYS			84.025		-13.965		20.00	6	
	MOTA	315	CE			111	84.318		-13.277		20.00	6	
	MOTA	316	NZ ·				83.784		-11.875		20.00	7	
	ATOM	317	C	LYS			85.844		-17.869		20.00	6	
·55	MOTA	318	0	LYS			86.017		-17.688		20.00	8 7	•
	ATOM	319	N			112	85.078		-18.838		20.00	6	
	ATOM	320	CA			112	84.383		-19.782 -21.233		20.00	6	
	MOTA	321	CB			112	84.695		-21.233		20.00	6	
	ATOM	322	CG2	ILE	B	. 117	84.042	33.303	22.210	1.00	20.00	•	

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MOTA
              323
                   CG1 ILE B 112
                                        86.216
                                                 34.518 -21.440
                                                                  1.00 20.00
                                                                                6
     MOTA
              324
                   CD1 ILE B 112
                                        86.657
                                                 33.949 -22.779
                                                                  1.00 20.00
                                                                                6
     ATOM
              325
                        ILE B 112
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                                                 34.916 -19.538
                   С
                                                                  1.00 20.00
                                                                                6
              326
                                                 33.839 -19.510
     MOTA
                   0
                        ILE B 112
                                        82.288
                                                                  1.00 20'.00
                                                                                8
              327
                                                 36.083 -19.347
     ATOM
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                        LEU B 113
                                        82.269
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              328
                        LEU B 113
                                        80.835
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                                                 36.038 -16.521
                   CG
                        LEU B 113
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                   CD1 LEU B 113
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              332
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                   CD2 LEU B 113
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                                        80.172
                                                 37.110 -20.090
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                        LEU B 113
                   С
                                                                  1.00 20.00
                                                                                6
                        LEU B 113
     ATOM
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                                        79.088
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     ATOM
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                        GLU B 114
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                                                 40.808 -20.553
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                                                                               6
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                                                                               6
25
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                        LYS B 115
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                        HIS B 117
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                        HIS B 117
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45
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                                                                               6
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50
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                        ILE B 118
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ILE B 119
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                                                 40.349 -17.690
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                        ILE B 119
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	ATOM	501		ASP		•	81.739	45.167	-5.747		20.00	. 8
	ATOM	502	C	ASP			85.192	41.969	-4.401		20.00	6
	ATOM	503	ŏ		_	132	86.191	42.337	-3.783		20.00	8
5	ATOM	504	N	VAL			84.596	40.809	-4.150		20.00	7
,	ATOM	505	CA	VAL			85.131	39.933	-3.116		20.00	6
	ATOM	506	CB	VAL			84.226	38.698	-2.885		20.00	6
	ATOM	507		VAL			84.920	37.713	-1.957		20.00	6
	ATOM	508		VAL			82.893	39.135	-2.271		20.00	6
10	ATOM	509	C	VAL			86.540	39.470	-3.477		20.00	6
10		510	0	VAL			87.460	39.602	-2.675		20.00	8
•	ATOM	511	N	MET		134	86.721	38.950	-4.688		20.00	7
	ATOM ATOM	512	CA	MET			88.040	38.474	-5.083		20.00	6
	ATOM	513	CB	MET			88.004	37.879	-6.492		20.00	6
15	ATOM	514	CG	MET		134	87.183	36.603	-6.573		20.00	6
13		514	SD	MET				35.650			20.00	16
	ATOM	516	CE	MET		134	87.477		-8.077 -7.475			
	ATOM	517		MET			88.730 89.115	34.515 39.552	-7.475 -4.994		20.00	6
	ATOM	518	C O	MET		134	90.253	39.332	-4.626		20.00	6 8
20	ATOM	519	N	SER			88.758	40.790	-5.319		20.00	7
20	ATOM ATOM	520	CA	SER			89.708	41.899	-5.260		20.00	6
	MOTA	521	CB	SER			89.084	43.175	-5.836		20.00	6
	ATOM	522	OG	SER			88.742	43.009	-7.202		20.00	8
	ATOM	523	C	SER			90.165	42.184	-3.830		20.00	6
25	ATOM	524	o	SER			91.228	42.762	-3.614		20.00	8
23	ATOM	525	N	ARG			89.354	41.782	-2.857		20.00	7
	ATOM	526	CA	ARG			89.672	42.013	-1.450		20.00	6
	ATOM	527	CB	ARG			88.384	42.156	-0.637		20.00	6
	ATOM	528	CG	ARG		136	87.509	43.336	-1.018		20.00	6
30	ATOM	529	CD			136 .	86.215	43.306	-0.211		20.00	6
	ATOM	530	NE	ARG		136	86.491	43.117	1.209		20.00	7
	ATOM	531	CZ	ARG			85.565	42.888	2.132		20.00	6
	ATOM	532	NH1	ARG	В	136	84.285	42.821	1.786	1.00	20.00	7
	ATOM	533	NH2	ARG	В	136	85.920	42.715	3.401	1.00	20.00	7
35	ATOM	534	С	ARG	В	136	90.506	40.891	-0.839	1.00	20.00	6
	ATOM	535	0	ARG	В	136	91.091	41.054	0.231	1.00	20.00	8
	ATOM	536	N	LEU	В	137	90.556	39.752	-1.515	1.00	20.00	7
	ATOM	537	CA	LEU	В	137	91.300	38.609	-1.005	1.00	20.00	6
	MOTA	538	CB	LĘU	В	137	90.665	37.307	-1.504	1.00	20.00	6
40	MOTA	539	CG	LEU	В	137	89.172	37.099	-1.213	1.00	20.00	6
	ATOM	540	CD1	LEU	В	137	88.748	35.728	-1.734	1.00	20.00	6
	ATOM	541	CD2	LEU	В	137	88.897	37.205	0.280	1.00	20.00	. 6
	ATOM	542	С	LEU		137	92.771	38.648	-1.402		20.00	6
	ATOM	543	0	LEU	В	137	93.103	38.871	-2.566	1.00	20.00	8
45	ATOM	544	N	ASP			93.645	38.436	-0.424		20.00	7
	MOTA	545	CA	ASP			95.086	38.422	-0.656		20.00	6
	ATOM	546	CB	ASP			95.696	39.797	-0.352		20.00	6
	ATOM	547	CG	ASP			97.179	39.854	-0.674		20.00	6
	ATOM	548		ASP			97.601	39.173	-1.634		20.00	8
50	MOTA	549		ASP			97.920	40.581	0.022		20.00	8
	ATOM	550	С	ASP			95.678	37.369	0.263		20.00	6`
	ATOM	551	0	ASP			96.353	37.685	1.243		20.00	8
	ATOM	552	N	HIS			95.410	36.111	-0.065		20.00	7
	ATOM	553	CA	HIS			95.871	34.984	0.731		20.00	6
55	ATOM	554	СВ	HIS			94.769	34.610	1.737		20.00	6
	MOTA	555	CG	HIS			95.173	33.561	2.725		20.00	6
	MOTA	556		HIS			95.543	33.657	4.025		20.00	6
	ATOM	557		HIS			95.241	32.221	2.405		20.00	7
	ATOM	558	CEI	HIS	B	133	95.635	31.537	3.466	1.00	20.00	6

	ATOM	559	NE2	HIS			95.825	32.385	4.461	1.00 20	0.00	7
	ATOM	560	С	HIS	В	139	96.176	33.828	-0.221	1.00 20	00.0	6
	MOTA	561	0	HIS	В	139	95.444	33.595	-1.182	1.00 20	00.0	8
	ATOM	562	N	PRO	В	140	97.257	33.080	0.038	1.00 20	00.	7
5	ATOM	563	CD	PRO	В	140	98.128	33.140	1.225	1.00 20	00.0	6
	ATOM	564	CA	PRO	В	140	97.635	31.959	-0.827	1.00 20	00.0	6
	ATOM	565	CB	PRO	В	140	98.913	31.433	-0.171	1.00 20	.00	6
	ATOM	566	CG	PRO	В	140	98.687	31.730	1.277	1.00 20	.00	6
	ATOM	567	С			140	96.614	30.846	-1.072	1.00 20	.00	6
10	ATOM	568	0	PRO	В	140	96.747	30.107	-2.044	1.00 20	.00	8
	ATOM	569	N	PHE	В	141	95.607	30.712	-0.211	1.00 20	.00	7
	ATOM	570	CA	PHE	В	141	94.620	29.649	-0.398	100 20	.00	6
	ATOM	571	CB	PHE	В	141	94.206	29.056	0.961	1.00 20	.00	6
	MOTA	572	CG	PHE	В	141	95.321	28.335	1.681	1.00 20	.00	6
15	ATOM	573	CD1	PHE	В	141	96.351	27.716	0.967	1.00 20	.00	6
	ATOM	574	CD2	PHE	В	141	95.311	28.227	3.067	1.00 20	.00	6
	ATOM	575		PHE			97.350	27.000	1.627	1.00 20	.00	6
	MOTA	576	CE2	PHE	В	141	96.307	27.510	3.740	1.00 20	.00	6
	ATOM	577	CZ	PHE	В	141	97.328	26.895	3.018	1.00 20	.00	6
20	ATOM	578	С	PHE			93.371	30.063	-1.181	1.00 20	.00	6
	MOTA	579	0	PHE	В	141	92.335	29.398	-1.114	1.00 20	.00	8
	ATOM	580	N	PHE	В	142	93.471	31.150	-1.934	1.00 20	.00	7
	ATOM	581	CA	PHE			92.337	31.625	-2.721	1.00 20	.00	6
	ATOM	582	CB	PHE	В	142	91.739	32.883	-2.082	1.00 20	.00	6
25	ATOM	583	CG	PHE	В	142	91.048	32.628	-0.772	1.00 20	.00	6
	ATOM	584	CD1	PHE	В	142	89.715	32.227	-0.740	1.00 20	.00	6
	ATOM	585	CD2	PHE	В	142	91.741	32.747	0.429	1.00 20	.00	6
	ATOM	586	CE1	PHE	В	142	89.080	31.944	0.472	1.00 20	.00	6
	ATOM	587	CE2	PHE	В	142	91.116	32.465	1.647	1.00 20	.00	6
30	ATOM	588	CZ	PHE	В	142	89.785	32.064	1.667	1.00 20	.00	6
	MOTA	589	С	PHE	В	142	92.758	31.945	-4.146	1.00 20	.00	6
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	ATOM	591	N	VAL	В	143	91.883	31.653	-5.106	1.00 20	.00	7
	ATOM	592	CA	VAL	В	143	92.167	31.960	-6.504	1.00 20	.00	6
35	ATOM	593	CB	VAL	В	143	91.009	31.513	-7.435	1.00 20	.00	6
	MOTA	594	CG1	VAL	В	143	91.116	32.209	-8.795	1.00 20	.00	6
	ATOM	595	CG2	VAL	В	143	91.061	30.000	-7.623	1.00 20	.00	6
	MOTA	596	С	VAL	Ė	143	92.301	33.469	-6.545	1.00 20	.00	6
	ATOM	597	0	VAL	В	143	91.505	34.179	-5.932	1.00 20		8
40	ATOM	598	N	LYS	В	144	93.312	33.957	-7.252	1.00 20	.00	7
	ATOM	599	CA	LYS	В	144	93.547	35.392	-7.340	1.00 20	.00	6
	ATOM	600	CB	LYS	В	144	95.051	35.689	-7.267	1.00 20	.00	6
	ATOM	601	CG	LYS	В	144	95.382	37.182	-7.318	1.00 20	.00	6
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50	MOTA	608	CA	LEU	В	145	91.968	37.975	-9.624	1.00 20	.00	6
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55	MOTA	613	С	LEU	В	145	93.059	38.984	-9.968	1.00 20	.00	6
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	ATOM	798	CG	LEU			89.408	18.363	-2.569	1.00 20.00	6
5	ATOM	799		LEU			90.769	17.703	-2.412	1.00 20.00	6
•	ATOM	800		LEU			89.065	19.193	-1.338	1.00 20.00	6
	ATOM	801	С	LEU			88.757	17.394	-5.346	1.00 20.00	6
	ATOM	802	Ō	LEU			89.124	16.283	-4.968	1.00 20.00	8
	ATOM	803	N	LEU			87.580	17.600	-5.927	1.00 20.00	7
10	ATOM	804	CA	LEU			86.647	16.500	-6.153	1.00 20.00	6
	ATOM	805	CB	LEU			85.364	17.014	-6.809	1.00 20.00	6
	ATOM	806	CG	LEU			84.292	15.977	-7.168	1.00 20.00	6
	ATOM	807		LEU	В	168	83.883	15.186	-5.929	1.00 20.00	6
	ATOM	808	CD2	LEU	В	168	83.083	16.687	-7.756	1.00 20.00	6
15	ATOM	809	С	LEU			87.290	15.440	-7.046	1.00 20.00	6
	ATOM	810	0	LEU	В	168	87.091	14.243	-6.845	1.00 20.00	8
	ATOM	811	N	LYS	В	169	88.068	15.888	-8.027	1.00 20.00	7
	ATOM	812	CA	LYS	В	169	88.727	14.967	-8.941	1.00 20.00	6
	ATOM	813	СВ			169	89.610	15.729	-9.930	1.00 20.00	6
20	ATOM	814	CG	LYS	В	169	90.379	14.818	-10.882	1.00 20.00	6
	MOTA	815	CD	LYS	В	169	91.226	15.603	-11.877	1.00 20.00	6
	ATOM	816	CE	LYS	В	169	92.373		-11.192	1.00 20.00	6
	ATOM	817	NZ	LYS	В	169	93.253		-12.173	1.00 20.00	7
	ATOM	818	С	LYS	В	169	89.574	13.949	-8.193	1.00 20.00	6
25	ATOM	819	0			169	89.543	12.758	-8.504	1.00 20.00	8
	ATOM	820	N	TYR	В	170	90.334	14.417	-7.207	1.00 20.00	7
	ATOM	821	CA			170	91.197	13.527	-6.441	1.00 20.00	6
	ATOM	822	CB			170	92.243	14.346	-5.682	1.00 20.00	6
	ATOM	823	CG			170	93.217	15.010	-6.624	1.00 20.00	6
30	ATOM	824		TYR			94.347	14.331	-7.085	1.00 20.00	6
	MOTA	825		TYR			95.195	14.900	-8.036	1.00 20.00	6
	ATOM	826		TYR			92.963	16.282	-7.133	1.00 20.00	6
	ATOM	827		TYR		170	93.801	16.861	-8.083	1.00 20.00	6 6
	ATOM	828	CZ			170	94.913	16.164	-8.532	1.00 20.00	8
35	ATOM	829	OH			170	95.727	16.727	-9.493	1.00 20.00	6
	ATOM	830	С			170	90.419	12.622	-5.499	1.00 20.00 1.00 20.00	8
	ATOM	831	0			170	90.834	11.494	-5.233 -4.993	1.00 20.00	7
	ATOM	832	N			171	89.287	13.098	-4.993 -4.112	1.00 20.00	6
40	ATOM	833	CA			171	88.488	12.262	-3.538	1.00 20.00	6
40	ATOM	834	CB			171	87.278 86.367	13.028 12.065	-2.791	1.00 20.00	6
	ATOM	835	CG2	ILE		171	87.764	14.141	-2.603	1.00 20.00	6
	ATOM	836	CG1	ILE			86.652	14.191	-2.019	1.00 20.00	6
	ATOM	837 838	CDI			171	87.994	11.066	-4.931	1.00 20.00	6
15	ATOM	839		ILE			88.030	9.925	-4.468	1.00 20.00	8
45	ATOM	840	N			172	87.550	11.331	-6.156	1.00 20.00	7
	ATOM ATOM	841	CA			172	87.061	10.273	-7.031	1.00 20.00	6
•	ATOM	842	CB			172	86.359	10.861	-8.259	1.00 20.00	6
	ATOM	843	CG			172	85.094	11.658	-7.963	1.00 20.00	6
50	ATOM	844	CD			172	84.352	11.981	-9.259	1.00 20.00	6
50	ATOM	845	NE			172	83.187	12.843	-9.063	1.00 20.00	
	ATOM	846	CZ			172	82.192	12.589	-8.217	1.00 20.00	6
	ATOM	847		ARG			82.209	11.491	-7.469	1.00 20.00	7
	ATOM	848		ARG			81.168	13.428	-8.127	1.00 20.00	7
55	ATOM	849	С			172	88.202	9.378	-7.497	1.00 20.00	6
	ATOM	850	ō			172	88.050	8.160	-7.587	1.00 20.00	8
	ATOM	851	N			173	89.348	9.985	-7.783	1.00 20.00	7
	ATOM	852	CA			173	90.509	9.244	-8.256	1.00 20.00	6
	ATOM	853	СВ			173	91.647	10.206	-8.603	1.00 20.00	6

	•											
	MOTA	854	CG	LYS	B 17	3		92.930	9.511	-9.045	1.00 20.00	
	ATOM	855	CD	LYS	B 17	3		94.081	10.496	-9.222	1.00 20.00	6 (
	ATOM	856	CE	LYS	B 17	3		93.862	11.432	-10.406	1.00 20.00) 6
	ATOM	857	NZ	LYS	B 17	3		93.858	10.711	-11.715	1.00 20.00	
5	ATOM	858	С	LYS	B 17	3		91.025	8.191	-7.280	1.00 20.00	6
	ATOM	859	O		B 17			91.274	7.055	-7.674	1.00 20.00	
	ATOM	860	N		B 17			91.192	8.554	-6.012	1.00 20.00	
	ATOM	861	CA	ILE		-		91.710	7.593	-5.042	1.00 20.00	
	ATOM	862	CB	ILE				92.884	8.191	-4.223	.1.00 20.00	
10	ATOM	863	CG2					93.970	8.701	-5.166	1.00 20.00	
10				ILE					9.337	-3.100		
	ATOM	864						92.394			1.00 20.00	
	ATOM	865	CD1					93.480	9.916	-2.457	1.00 20.00	
	ATOM	866	C	-	B 17			90.674	7.030	-4.074	1.00 20.00	
	ATOM	867	0	ILE				91.025	6.296	-3.151	1.00 20.00	
15	ATOM	868	N	GLY				89.405	7.367	-4.283	1.00 20.00	
	ATOM	869	CA		B 17			88.359	6.855	-3.413	1.00 20.00	
	ATOM	870	C	GLY				88.160	7.650	-2.138	1.00 20.00	
	ATOM	871	0	GLY	B 17	5		87.083	8.198	-1.905	1.00 20.00	
	ATOM	872	N	SER	в 17	6		89.192	7.701	-1.304	1.00 20.00	7
20	ATOM	873	CA	SER	B 17	6		89.140	8.447	-0.053	1.00 20.00	6
	ATOM	874	CB	SER	B 17	6		88.395	7.653	1.026	1.00 20.00	6
	ATOM	875	OG	SER	в 17	6		89.150	6.543	1.472	1.00 20.00	8
	ATOM	876	С	SER	в 17	6		90.565	8.742	0.401	1.00 20.00	6
	ATOM	877	0	SER	в 17	6		91.506	8.049	0.009	1.00 20.00	8
25	ATOM	878	N	PHE				90.718	9.769	1.228	1.00 20.00	
	ATOM	879	CA	PHE				92.029	10.184	1.722	1.00 20.00	
	ATOM	880	СВ	PHE				92.028	11.694	1.990	1.00 20.00	
	ATOM	881	·CG	PHE				92.002	12.546	0.747	1.00 20.00	
	ATOM	882		PHE				91.484	12.060	-0.449	1.00 20.00	
30	ATOM	883	CD2					92.481	13.855	0.787	1.00 20.00	
50	ATOM	884		PHE				91.443	12.860	-1.585	1.00 20.00	
		885		PHE				92.444	14.665	-0.343	1.00 20.00	
	ATOM										1.00 20.00	
	ATOM	886	CZ		B 17			91.925	14.168	-1.532		
25	ATOM	887	C	PHE				92.427	9.475	3.009	1.00 20.00	
35	ATOM	888	0	PHE				91.582	9.223	3.872	1.00 20.00	
	ATOM	889	N	ASP				93.711	9.152	3.147	1.00 20.00	
	MOTA	890	CA	ASP				94.155	8.529	4.385	1.00 20.00	
	MOTA	891	CB	ASP				95.581	7.972	4.267	1.00 20.00	
	ATOM	892	CG	ASP				96.594	9.018	3.845	1.00 20.00	
40	ATOM	893		ASP				96.392	10.214	4.139	1.00 20.00	
	ATOM	894		ASP				97.612	8.634	3.230	1.00 20.00	
	ATOM	895	С	ASP				94.092	9.640	5.436	1.00 20.00	
•	ATOM	896	0	ASP	в 17	8		93.736	10.778	5.117	1.00 20.00	
	ATOM	897	N	GLU	B 17	9		94.443	9.324	6.677	1.00 20.00	
45	ATOM	898	CA	GLU	B 17	9		94.380	10.311	7.744	1.00 20.00	6
	MOTA	899	CB	GLU	B 17	9		94.623	9.637	9.096	1.00 20.00	6
	ATOM	900	CG	GLU	B 17	9		94.747	10.611	10.255	1.00 20.00	6
	MOTA	901	CD	GLU	B 17	9		94.331	9.994	11.574	1.00 20.00	6
	ATOM	902	OE1	GLU	B 17	9		94.589	8.789	11.770	1.00 20.00	
50	ATOM	903		GLU				93.753	10.717	12.416	1.00 20.00	8
	ATOM	904	С	GLU				95.320	11.501	7.575	1.00 20.00	
	ATOM	905	ō	GLU				94.948	12.636	7.881	1.00 20.00	
	ATOM	906	N	THR				96.528	11.246	7.086	1.00 20.00	
	ATOM	907	CA	THR				97.509	12.308	6.886	1.00 20.00	
55	ATOM	908	CB	THR			•	98.866	11.720	6.445	1.00 20.00	
22	ATOM	909	OG1					99.349	10.842	7.466	1.00 20.00	
											1.00 20.00	
	ATOM	910		THR				99.888	12.825	6.213		
	ATOM	911	C	THR				97.040	13.331	5.849	1.00 20.00	
	ATOM	912	0	THR	р ТЯ	U		97.136	14.542	6.069	1.00 20.00	8

	ATOM	913	N	CYS	В	181	96.534	12.845	4.721	1.00 20.	00 7
	ATOM	914	CA	CYS	В	181	96.057	13.733	3.666	1.00 20.0	
	ATOM	915	СВ	CYS	В	181	95.836	12.945	2.375	1.00 20.	
	ATOM	916	SG	CYS	В	181	97.372	12.255	1.685	1.00 20.0	
5	ATOM	917	С			181	94.775	14.449	4.079	1.00 20.0	
_	ATOM	918	ō			181	94.570	15.615	3.733	1.00 20.0	
	ATOM	919	N		_	182	93.914	13.755	4.820	1.00 20.0	
	ATOM	920	CA			182	92.669	14.356	5.286	1.00 20.0	
	ATOM	921	CB	THR			91.812	13.354	6.103		-
10	ATOM	922	OG1							1.00 20.0	
10	ATOM	923					91.372	12.283	5.259	1.00 20.0	
		923	CG2				90.600	14.054	6.690	1.00 20.0	
	ATOM		C	THR			93.014	15.535	6.196	1.00 20.0	
	ATOM	925	0	THR			92.515	16.649	6.019	1.00 20.0	
1.5	MOTA	926	И.	ARG			93.873	15.273	7.175	1.00 20.0	
15	ATOM	927	CA	ARG			94.299	16.293	8.121	1.00 20.0	
	MOTA	928	СВ	ARG			95.311	15.707	9.109	1.00 20.0	
	ATOM	929	CG	ARG		183	95.957	16.744	10.012	1.00 20.0	0 6
	ATOM	930	CD	ARG	В	183	96.886	16.116	11.050	1.00 20.0	0 6
	ATOM	931	NE	ARG	В	183	96.167	15.220	11.949	1.00 20.0	0 7
20	MOTA	932	CZ	ARG	В	183	96.098	13.900	11.804	1.00 20.0	0 6
	ATOM	933	NH1	ARG	В	183	96.717	13.306	1,0.791	1.00 20.0	0 7
	ATOM	934	NH2	ARG	В	183	95.389	13.176	12.664	1.00 20.0	0 7
	ATOM	935	C-	ARG	В	183	94.923	17.505	7.427	1.00 20.0	0 6
•	ATOM	936	0	ARG	В	183	94.545	18.646	7.698	1.00 20.0	0 8
25	ATOM	937	N	PHE	В	184	95.877	17.264	6.534	1.00 20.0	0 7
	ATOM	938	CA	PHE	В	184	96.539	18.367	5.847	1.00 20.0	
	ATOM	939	CB	PHE	В	184	97.610	17.847	4.889	1.00 20.0	
	ATOM	940	CG	PHE	В	184	98.387	18.943	4.223	1.00 20.0	
	ATOM	941		PHE	В	184	99.451	19.555	4.879	1.00 20.0	
30	ATOM	942		PHE			98.009	19.415	2.975	1.00 20.0	
	ATOM	943		PHE			100.125	20.627	4.301	1.00 20.0	
	ATOM	944		PHE		184	98.676	20.491	2.388	1.00 20.0	
	ATOM	945	CZ	PHE			99.735	21.097	3.053	1.00 20.0	
	ATOM	946	C	PHE			95.580	19.267	5.066	1.00 20.0	
35	ATOM	947	Ö	PHE		184	95.567	20.481	5.255	1.00 20.0	
23	ATOM	948	N	TYR			94.784	18.679	4.181	1.00 20.0	
	ATOM	949	CA	TYR			93.854	19.471	3.390	1.00 20.0	-
	ATOM	950	CB	TYR		185	93.305	18.634	2.236	1.00 20.0	•
	ATOM	951	CG	TYR			94.337	18.504		1.00 20.0	
40	ATOM	952	CD1				94.611	19.580	0.293	1.00 20.0	-
70				TYR			95.637				
	ATOM ATOM	953 954		TYR			95.118	19.516 17.352	-0.643 1.017	1.00 20.0	
		955									
	MOTA		CE2			-	96.152	17.282	0.081	1.00 20.0	
15	ATOM	956	CZ	TYR			96.405	18.367	-0.742	1.00 20.0	
45	ATOM	957	OH	TYR			97.436	18.314	-1.657	1.00 20.0	
	ATOM	958	С	TYR			92.738	20.098	4.208	1.00 20.0	
	MOTA	959	0	TYR			92.286	21.195	3.891	1.00 20.0	
	MOTA	960	N	THR			92.303	19.422	5.267	1.00 20.0	
	MOTA	961	CA	THR				19.987	6:122	1.00 20.0	
50	MOTA	962	CB	THR			. 90.799	18.996	7.219	1.00 20.0	
	ATOM	963		THR			90.193	17.846	6.606	1.00 20.0	
	MOTA	964		THR			89.774	19.671	8.144	1.00 20.0	
	MOŢA	965	С	THR			91.858	21.218	6.805	1.00 20.0	
	MOTA	966	0	THR			91.188	22.242	6.948	1.00 20.0	
55	MOTA	967	N	ALA			93.120	21.115	7.222	1.00 20.0	
	MOTA	968	CA	ALA			93.787	22.234	7.882	1.00 20.0	
	ATOM	969	СВ	ALA			95.184	21.817	8.349	1.00 20.0	0 6
	ATOM	970	С	ALA	В	187	93.879	23.449	6.946	1.00 20.0	0 6
	ATOM	971	0	ALA	В	187	. 93.654	24.585	7.372	1.00 20.0	8 0

												_
	ATOM	972 .	N	GLU				94.205	23.222	5.674	1.00 20.00	7
•	ATOM	973	CA	GLU				94.292	24.343	4.740	1.00 20.00	6
	ATOM	974	CB	GLU	В	188		94.843	23.898	3.376	1.00 20.00	6
	ATOM	975	CG	GLU	В	188		96.285	23.391	3.407	1.00 20.00	6
5	ATOM	976	CD	GLU	В	188.		97.030	23.639	2.104	1.00 20.00	6
	ATOM	977	OE1	GLU	В	188		96.407	23.537	1.024	1.00 20.00	8
	ATOM	978	OE2	GLU	В	188		98.247	23.932	2.156	1.00 20.00	8
	ATOM	979	С	GLU	В	188		92.912	24.977	4.561	1.00 20.00	6
	ATOM	980	0	GLU	В	188		92.782	26.196	4.533	1.00 20.00	8
10	ATOM	981	N	ILE	В	189		91.875	24.152	4.451	1.00 20.00	7
	ATOM	982	CA	ILE				90.530	24.693	4.284	1.00 20.00	6
	ATOM	983	СВ	ILE	В	189		89.495	23.566	4.064	1.00 20.00	6
	ATOM	984		ILE	в	189		88.094	24.157	3.947	1.00 20.00	6
	ATOM	985	CG1	ILE				89.855	22.773	2.796	1.00 20.00	6
15	ATOM	986	CD1	ILE				89.058	21.488	2.616	1.00 20.00	
13	ATOM	987	C	ILE				90.152	25.517	5.519	1.00 20.00	6
	ATOM	988	o	ILE				89.634	26.630	5.396	1.00 20.00	8
		989	N	VAL				90.412	24.971	6.707	1.00 20.00	7
	ATOM	990	CÀ	VAL				90.116	25.674	7.957	1.00 20.00	6
20	ATOM	991	CB	VAL				90.557	24.842	9.186	1.00 20.00	6
20	MOTA			VAL				90.540	25.717	10.451	1.00 20.00	6
	ATOM	992 993		VAL				89.643	23.641	9.358	1.00 20.00	6
	MOTA			VAL				90.865	27.012	7.984	1.00 20.00	6
	ATOM	994	C	VAL				90.311	28.039	8.375	1.00 20.00	8
0.5	ATOM	995	0	SER				92.125	26.997	7.557	1.00 20.00	7
25	ATOM	996	N					92.123	28.218	7.546	1.00 20.00	6
	ATOM	997	CA	SER					27.888	7.166	1.00 20.00	6
	ATOM	998	CB			191	•	94.378 95.220	29.007	7.363	1.00 20.00	8
	ATOM	999	OG	SER				92.361	29.240	6.566	1.00 20.00	6
	ATOM	1000	С	SER					30.444	6.838	1.00 20.00	8
30	ATOM	1001	0	SER				92.351	28.754	5.425	1.00 20.00	7
	ATOM	1002	N	ALA				91.882			1.00 20.00	6
	MOTA	1003	CA	ALA				91.306	29.634. 28.850	3.141	1.00 20.00	6
	ATOM	1004	CB	ALA				91.006	30.256	4.970	1.00 20.00	6
	MOTA	1005	C	ALA				90.029		4.822	1.00 20.00	8
35	ATOM	1006	0	ALA				89.799	31.458	5.621	1.00 20.00	7
	ATOM	1007	N	LEU				89.203	29.439		1.00 20.00	6
	ATOM	1008	CA	LEU				87.957	29.941	6.192 6.725	1.00 20.00	6
	ATOM	1009	CB	LEU				87.101	28.783	5.650	1.00 20.00	6
	MOTA	1010	CG	LEU				86.447	27.898	6.315	1.00 20.00	6
40	ATOM	1011		LEU				85.645	26.771	4.780	1.00 20.00	6
	ATOM	1012		LEU				85.530	28.752	7.299	1.00 20.00	6
	ATOM	1013	С	LEU				88.215	30.959		1.00 20.00	8
	ATOM	1014	0	LEU		193		87.474	31.935	7.435 8.100	1.00 20.00	
	ATOM	1015	N	GLU	_			89.254	30.738	9.157	1.00 20.00	
45	ATOM	1016	CA	GLU				89.562			1.00 20.00	
	ATOM	1017	CB	GLU				90.773	31.257	9.982		6
	ATOM	1018	CG	GLU				91.288	32.353	10.914	1.00 20.00	
	ATOM	1019	CD	GLU				92.381	31.878	11.855	1.00 20.00	
	ATOM	1020		GLU				93.246	31.090	11.420	1.00 20.00	
50	ATOM	1021		GLU				92.376	32.312	13.031	1.00 20.00	
	MOTA	1022	С	GLU			•	89.847	33.053	8.511	1.00 20.00	
	MOTA	1023	0	GLU				89.375	34.083	8.972	1.00 20.00	
	MOTA	1024	N			195		90.608	33.046	7.426	1.00 20.00	
	ATOM	1025	CA			195		90.928	34.294	6.743	1.00 20.00	
55	ATOM	1026	CB			195		91.919	34.043	5.613	1.00 20.00	
	ATOM	1027	CG			195		92.193	35.271	4.774	1.00 20.00	
	ATOM	1028		TYR				93.098	36.244	5.202	1.00 20.00	
•	ATOM	1029	CE1	TYR	В	195		93.356	37.382	4.429	1.00 20.00	
	ATOM	1030	CD2	TYR	В	195		91.545	35.461	3.553	1.00 20.00	6

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             1031
                    CE2 TYR B 195
                                         91.794
                                                  36.591
                                                           2.775
                                                                   1.00 20.00
     ATOM
             1032
                    CZ
                        TYR B 195
                                         92.701
                                                  37.545
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     MOTA
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                                         92.956
                    OH
                        TYR B 195
                                                  38.656
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     ATOM
             1034
                         TYR B 195
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                    C
                                                  34.923
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             1035
                        TYR B 195
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                                                  34.103
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                        LEU B 196
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                        LEU B 196
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                        LEU B 196
                                         85.933
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     ATOM
             1040
                    CD1 LEU B 196
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                                                 34.659
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     ATOM
             1041
                    CD2 LEU B 196
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                                                 32.568
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                                                                   1.00 20.00
                                                                                6
     ATOM
             1042
                        LEU B 196
                                         86.731
                                                 35.161
                    С
                                                           5.888
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                                                                                6
                                                 36.308
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             1043
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                        LEU B 196
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                        HIS B 197
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                                         86.431
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15
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                        HIS B 197
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                    CA
                                                 34.840
                                                           7.967
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                                        85.241
     ATOM
             1046
                        HIS B 197
                    CB
                                                 33.697
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             1047
                        HIS B 197
                    CG
                                        84.377
                                                 32.622
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                                                           8.356
                                                                                6
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             1048
                    CD2 HIS B 197
                                        83.734
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                    ND1 HIS B 197
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             1049
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                                                 31.452
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20
     ATOM
             1050
                    CE1 HIS B 197
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                    NE2 HIS B 197
                                        83.071
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                                                                   1.00 20.00
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                    C
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                        GLY B 198
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                                                                                7
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                        GLY B 198
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                                                 37.285
                    ÇA
                                                           9.464
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     MOTA
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                        GLY B 198
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                                                 38.580
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                                                           8.737
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                        GLY B 198
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                                                 39.661
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                                                                   1.00 20.00
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                        LYS B 199
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     ATOM
             1059
                        LYS B 199
                   CA
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                                                 39.652
                                                           6.674
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30
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                   CB
                        LYS B 199
                                        87.577
                                                 39.573
                                                           5.279
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     MOTA
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                   CG
                        LYS B 199
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                        LYS B 199
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                   CE
                       LYS B 199
                                        91.054 40.243
                                                           3.807
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     ATOM
             1064
                   NZ LYS B 199
                                                 41.382
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                        LYS B 199
                                        85.451
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                                                                  1.00 20.00
                   C
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             1066
                        LYS B 199
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                        GLY B 200
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     ATOM
             1068
                       GLY B 200
                                        83.258
                   CA
                                                 39.158
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                                                                                6
                        GLY B 200
     ATOM
             1069
                   C
                                        82.646
                                                 38.660
                                                           6.032
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40 .
     ATOM
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                        GLY B 200
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                                      83.257
                                                 36.413
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81.125
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                                                          4.016
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                       ILE B 202
    ATOM
            1081
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                                                          4.481
                                                                  1.00 20.00
                                                                               6
    MOTA
                   CG2 ILE B 202
                                                32.522
            1082
                                        78.583
                                                          4.595
                                                                  1.00 20.00
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    ATOM
            1083
                   CG1 ILE B 202
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                                                34.675
                                                          5.825
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                                                34.865
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            1084
                   CD1 ILE B 202
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                                                                  1.00 20.00
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                                                                               6
55
                       ILE B 202
     ATOM
            1085
                   С
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                       ILE B 202
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                                                                  1.00 20.00
    ATOM
            1087
                   N
                       HIS B 203
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            1088
                       HIS B 203
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	ATOM	1090	CG	HIS	В	203		82.478	29.942	-0.380	1.00 20.00) 6
	ATOM	1091	CD2	HIS	В	203	•	81.646	29.282	-1.220	1.00 20.00	
	ATOM	1092		HIS				83.659	30.116	-1.069	1.00 20.00	
	ATOM	1093		HIS				83.545	29.588	-2.275	1.00 20.00	
5	ATOM	1094		HIS				82.333	29.076	-2.392	1.00 20.00	
•	ATOM	1095	С			203		79.896	31.211	0.530	1.00 20.00	
	ATOM	1096	ō			203		79.508	31.546	-0.593	1.00 20.00	
	ATOM	1097	N	ARG				79.168	30.458	1.357	1,00 20.00	
	ATOM	1098	CA	ARG				77.819	29.969	1.039	1.00 20.00	
10	ATOM	1099	CB	ARG		204		76.916	31.117	0.583	1.00 20.00	
10	ATOM	1100	CG	ARG								
				ARG				76.601		1.675	1.00 20.00	
	ATOM	1101	CD					75.316	32.878	1.377	1.00 20.00	
	ATOM	1102	NE	ARG		204		75.376	33.616	0.119	1.00 20.00	
1.5	ATOM	1103	CZ	ARG				74.423	34.443	-0.303	1.00 20.00	
15	ATOM	1104		ARG				73.336	34.636	0.436	1.00 20.00	
	ATOM	1105		ARG				74.555	35.084	-1.457	1.00 20.00	
	ATOM	1106	С	ARG				77.700	28.829	0.030	1.00 20.00	
	ATOM	1107	0	ARG				76.611	28.300	-0.177	1.00 20.00	
	ATOM	1108	N	ASP				78.792	28.456	-0.620	1.00 20.00	
20	MOTA	1109	CA	ASP				78.718	27.342	-1.550	1.00 20.00	
	ATOM	1110	CB	ASP				78.380	27.829	-2.961	1.00 20.00	
	ATOM	1111	CG	ASP	В	205		77.941	26.694	-3.867	1.00 20.00	6
	ATOM	1112	OD1	ASP	В	205		77.544	25.638	-3.330	1.00 20.00	8
	ATOM	1113	OD2	ASP	В	205		77.982	26.853	-5.104	1.00 20.00	
25	ATOM	1114	С	ASP	В	205		80.019	26.560	-1.547	1.00 20.00	6
	ATOM	1115	0	ASP	В	205	•	80.508	26.122	-2.588	1.00 20.00	8
	ATOM	1116	N	LEU	В	206		80.573	26.375	-0.354	1.00 20.00	7
	ATOM	1117	CA	LEU	В	206		81.819	25.652	-0.208	1.00 20.00	6
	ATOM	1118	CB	LEU	В	206		82.361	25.826	1.212	1.00 20.00	6
30	MOTA	1119	CG	LEU	В	206		83.764	25.271	1.471	1.00 20.00	'6
	ATOM	1120	CD1	LEU	В	206		84.765	25.969	0.561	1.00 20.00	
	ATOM .	1121	CD2	LEU	В	206		84.135	25.477	2.933	1.00 20.00	
	MOTA	1122	С	LEU				81.609	24.174	-0.514	1.00 20.00	6
	ATOM	1123	0	LEU				80.691	23.549	0.011	1.00 20.00	
35	ATOM	1124	N	LYS				82.461	23.628	-1.375	1.00 20.00	
	ATOM	1125	CA	LYS				82.379	22.223	-1.765	1.00 20.00	
	ATOM	1126	СВ	LYS				81.160	22.000	-2.679	1.00 20.00	
	ATOM	1127	CG	LYS				81.130	22.913	-3.893	1.00 20.00	
	ATOM	1128	CD	LYS				79.876	22.720	-4.736	1.00 20.00	
40	ATOM	1129	CE	LYS				79.788	23.797	-5.813	1.00 20.00	
	ATOM	1130	NZ	LYS				78.695	23.557	-6.791	1.00 20.00	
	ATOM	1131	C	LYS				83.657	21.808	-2.487	1.00 20.00	
	ATOM	1132	ŏ.	LYS				84.416	22.656	-2.960	1.00 20.00	
	ATOM	1133	N	PRO				83.916	20.494	-2.582	1.00 20.00	
45	ATOM	1134	CD	PRO				83.153	19.378	-1.993	1.00 20.00	ę ę
-13	ATOM	1135	CA	PRO				85.122	20.005	-3.259	1.00 20.00	6
	ATOM	1136	CB	PRO				84.922	18.494	-3.267	1.00 20.00	6
	ATOM	1137	CG	PRO				84.174	18.256	-1.984	1.00 20.00	. 6
	ATOM	1137	C	PRO				85.303	20.574	-4.666	1.00 20.00	. 6
50	ATOM	1139	0	PRO				86.431	20.752	-5.124	1.00 20.00	
30		1140		GLU							1.00 20.00	8 7
	ATOM		N					84.197	20.859	-5.347		
	ATOM	1141	CA	GLU				84.243	21.410	-6.705	1.00 20.00	6
	ATOM	1142	CB	GLU				82.836	21.424	-7.317	1.00 20.00	6
	ATOM	1143	CG	GLU				82.755	22.081	-8.690	1.00 20.00	6
55	ATOM	1144	CD	GLU				81.323	22.296	-9.159	1.00 20.00	6
	ATOM	1145		GLU				80.587	21.299	-9.322	1.00 20.00	8
	ATOM	1146		GLU				80.933	23.465	-9.364	1.00 20.00	8
	ATOM	1147	C	GLU				84.810	22.836	-6.716	1.00 20.00	6
	MOTA	1148	0	GLU	В	209		85.409	23.269	-7.705	1.00 20.00	8

	2001	1140	NT	A CNI	ъ	210	84.60	4 22 540	-5.612	1.00 20.	00	7
	ATOM	1149	N							1.00 20.		٠6
	MOTA	1150	CA			210						
	MOTA	1151	CB			210	84.03			1.00 20.		6
_	MOTA	1152	CG			210	82.85			1.00 20.		6
5	ATOM	1153		ASN			81.80			1.00 20.		8
	ATOM	1154		ASN			83.01			1.00 20.		7
	ATOM	1155	С			210	86.42			1.00 20.		6
	ATOM	1156	0	ASN	В	210	86.93	7 26.181		1.00 20.	00	8
	ATOM	1157	N	ILE	В	211	87.01			1.00 20.	00	7
10	ATOM	1158	CA	ILE	В	211	88.33	1 23.958	-3.790	1.00 20.	00	6
	ATOM	1159	CB	ILE	В	211	88.33	6 23.090	-2.521	1.00 20.	00	6
	ATOM	1160	CG2	ILE	В	211	89.73	2 23.025	-1.925	1.00 20.	00	6
	ATOM	1161	CG1	ILE	·B	211	87.35	0 23.682	-1.510	1.00 20.	00	6
	ATOM	1162		ILE			87.12			1.00 20.	00	6
15	ATOM	1163	C			211	89.30			1.00 20.		6
	ATOM	1164	ō			211	89.47			1.00 20.		8
	ATOM	1165	N			212	89.93		-	1.00 20.		7
	ATOM	1166	CÀ			212	90.87			1.00 20.		6
	ATOM	1167	CB			212	90.96			1.00 20.		6
20							89.63			1.00 20.		6
20	ATOM	1168	CG			212				1.00 20.		6
	MOTA	1169		LEU			89.89					6
	ATOM	1170		LEU			88.78			1.00 20.		
	ATOM	1171	С			212	92.25			1.00 20.		6
	ATOM	1172	0			212	92.53			1.00 20.		8
25	ATOM	1173	N			213	93.11			1.00 20.		7
	ATOM	1174	CA			213	94.47			1.00 20.		6
	MOTA	1175	CB			213	94.60			1.00 20.		6
1	MOTA	1176	CG			213	93.77			1.00 20.		6
		1177		LEU			93.73			1.00 20.		6
30	ATOM	1178	CD2	LEU			94.37	•		1.00 20.		6
	ATOM	1179	С			213	95.50	3 23.277		1.00 20.		6
	MOTA	1180	0	LEU	В	213	95.42			1.00 20.		8
	ATOM	1181	N	ASN	В	214	96.47		-6.940	1.00 20.		7 .
	ATOM	1182	CA	ASN	В	214	97.48	8 24.585	-7.826	1.00 20.	00	6
35	ATOM	1183	CB	ASN	В	214	98.19	8 25.792	-7.201	1.00 20.	00	6
	ATOM	1184	CG	ASN	В	214	98.93	8 25.448	-5.927	1.00 20.	00	6
	ATOM	1185	OD1	ASN	В	214	99.26	7 24.288	-5.669	1.00 20.	00	8
	ATOM	1186	ND2	ASN	В	214	99.22	4 26.4 <i>6</i> 9	-5.123	1.00 20.	00	7
	ATOM	1187	С	ASN	В	214	98.50	8 23.515	-8.182	1.00 20.	00	6
40	MOTA	1188	0	ASN	В	214	98.42	0 22.372	-7.725	1.00 20.	00	8
	ATOM	1189	N	GLU	В	215	99.48	2 23.894	-8.996	1.00 20.	00	7
	ATOM	1190	CA			215	100.51	4 22.965	-9.430	1.00 20.	00	6
	ATOM	1191	СВ	GLU	В	215	101.49		-10.362	1.00 20.	00	6
	ATOM	1192	CG			215	102.54		-10.979	1.00 20.	00	6
45	ATOM	1193		GLU					-12.080	1.00 20.	00	6
	ATOM	1194		GLU			103.90		-11.810	1.00 20.		8
	ATOM	1195		GLU			103.34		-13.215	1.00 20.		8
	ATOM	1196	C			215	101.27			1.00 20.		6
	ATOM	1197	Ö			215	101.80			1.00 20.		8
50	ATOM	1198				216	101.33			1.00 20.		7
50			N	ASP						1.00 20.		6
	ATOM	1199 1200	CA				102.03			1.00 20.		6
	ATOM		CB	ASP			102.72					
	ATOM	1201	CG			216	103.95		5.896	1.00 20,		6
	ATOM	1202		ASP			104.76			1.00 20.		8
5 5	ATOM	1203		ASP			104.110			1.00 20.		8
	ATOM	1204	C			216	101.12			1.00 20.		6
	MOTA	1205	0	ASP			101.53			1.00 20.		8
	MOTA	1206	N	MET			99.87			1.00 20.		7
	MOTA	1207	CA	MET	В	217	98.890	20.730	-4.657	1.00 20.	υU	6

	ATOM	1208	СВ	MET			99.402	19.319	-4.358		20.00	6
	ATOM	1209	CG	MET			99.456	18.432	-5.601		20.00	6
	ATOM	1210	SD	MET			97.857	18.342	-6.445		20.00	
	ATOM	1211	CE	MET			97.073	16.984	-5.543		20.00	6
5	ATOM	1212	С	MET			98.397	21.403	-3.373		20.00	6
	ATOM	1213	Ο.	MET			97.972	20.730	-2.435		20.00	8
	ATOM	1214	N	HIS			98.469	22.730	-3.331		20.00	7
	ATOM	1215	CA	HIS			97.949	23.487	-2.197		20.00	6
	ATOM	1216	CB	HIS			98.831	24.700	-1.898		20.00	6
10	MOTA	1217	CG	HIS			100.100	24.357	-1.177		20.00	6
	ATOM	1218	CD2	HIS	В	218	101.390	24.362	-1.588		20.00	6
	ATOM	1219		HIS			100.117	23.935	0.136		20.00	7
	ATOM	1220	CE1	HIS	В	218	101.364	23.698	0.504		20.00	6
	ATOM	1221	NE2	HIS	В	218	102.156	23.947	-0.524		20.00	7
15	ATOM	1222	С	HIS			96.583	23.939	-2.703		20.00	6
	ATOM	1223	0	HIS	В	218	96.400	24.090	-3.910		20,00	.8
	ATOM	1224	N	ILE	В	219	95.628	24.160	-1.808		20.00	7
	MOTA	1225	CA	ILE	В	219	94.301	24.562	-2.257		20.00	6
	ATOM	1226	CB	ILE			93.232	24.359	-1.159		20.00	6
20	ATOM	1227	CG2	ILE	В	219	93.266	22.918	-0.654			6
	ATOM	1228		ILE				. 25.353	-0.011		20.00	6
	ATOM	1229	CD1	ILE			92.351	25.342	1.036		20.00	6
	ATOM	1230	С	ILE	В	219	94.207	26.010	-2.714		20.00	6
	MOTA	1231	0	ILE	В	219	95.044	26.850	-2.375		20.00	8
25	ATOM	1232	N	GLN	В	220	93.168	26.274	-3.497		20.00	7
	ATOM	1233	CA	GLN	В	220	92.859	27.600	-3.999		20.00	6
	ATOM	1234	CB	GLN	В	220	93.537	27.867	-5.350		20.00	6
	ATOM	1235	CG			220	95.011	28.246	-5.216		20.00	6
	MOTA	1236	CD	GLN	В	220	95.599	28.799	-6.503		20.00	6
30	ATOM	1237		\mathtt{GLN}			95.725	28.086	-7.502		20.00	8
	ATOM	1238	NE2	GLN	В	220	95.957	30.079	-6.486		20.00	7
	ATOM	1239	С	GLN	В	220	91.350	27.626	-4.140		20.00	6
	MOTA	1240	0			220	90.792	27.133	-5.124		20.00	8
	ATOM	1241	N	ILE	В	221	90.689	28.178	-3.129		20.00	7
35	ATOM	1242	CA	ILE	В	221	89.240	28.260	-3.122		20.00	6
	ATOM	1243	CB			221	88.731	28.550	-1.700		20.00	6
	ATOM	1244	CG2	ILE	В	221	87.209	28.707	-1.708		20.00	6
	ATOM	1245	CG1				89.164	27.406	-0.773		20.00	6
	ATOM	1246	CD1	ILE	В	221	88.743	27.559	0.668		20.00	6
40	ATOM	1247	С			221	88.760	29.339	-4.092		20.00	6
	ATOM	1248	0	ILE	В	221	89.411	30.374	-4.262		20.00	8
	ATOM	1249	N	THR	·B	222	87.633	29.082	-4.748		20.00	7
	ATOM	1250	CA			222	87.084	30.039	-5.701		20.00	6
	ATOM	1251	CB	THR	В	222	87.565	29.728	-7.125		20.00	6
45	ATOM	1252		THR			87.179		-8.000			8
	MOTA	1253	CG2	THR			86.962	28.410	-7.618		20.00	6
	ATOM	1254	С	THR	В	222	85.554	30.028	-5.683		20.00	6
	ATOM	1255	0			222	84.950	29.417	-4.791		20.00	8
	ATOM	1256	N			223	84.949	30.712	-6.659		20.00	7
50	ATOM	1257	CA			223	83.492	30.806	-6.806		20.00	6
	ATOM	1258	CB			223	82.872	29.399	-6.767		20.00	6
	MOTA	1259	CG			223	81.414	29.384	-7.205		20.00	6
	ATOM	1260		ASP			80.990	30.335	-7.900		20.00	8
	ATOM	1261	OD2	ASP			80.701	28.414	-6.866		20.00	8
55	ATOM	1262	С			223	82.878	31.694	-5.725		20.00	6
	MOTA	1263	0			223	82.191	31.208	-4.820		20.00	8
	ATOM	1264	N			224	83.105	33.001	-5.848		20.00	7
	MOTA	1265	CA			224	82.632	33.970	-4.866		20.00	6
	MOTA	1266	CB	PHE	В	224	83.800	34.869	-4.451	1.00	20.00	6

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ATOM
                        PHE B 224
             1267
                   CG
                                        84.826
                                                 34,165
                                                         -3.612
                                                                  1.00 20.00
     ATOM
             1268
                   CD1 PHE B 224
                                                 33.931
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                                                         -2.261
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     ATOM
             1269
                   CD2 PHE B 224
                                        86.001
                                                 33.687
                                                         -4.182
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     MOTA
             1270
                   CE1 PHE B 224
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                                                 33.227
                                                         -1.486
                                                                  1.00 20.00
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     ATOM
             1271
                   CE2 PHE B 224
                                        86.927
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     MOTA
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                   CZ
                        PHE B 224
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                                        86.679
                                                 32.750
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             1273
                        PHE B 224
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                                                 34.839
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     ATOM
             1274
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                        PHE B 224
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                                                         -4.468
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                        GLY B 225
     MOTA
             1275
                   N
                                        80.928
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10
     MOTA
             1276
                   CA
                        GLY B 225
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                                                 35.438
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     ATOM
             1277
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                        GLY B 225
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                        THR B 226
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                        THR B 226
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15
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     ATOM
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                                                 32.417
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                                                                  1.00 20.00
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     MOTA
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                        THR B 226
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                                                         -2.981
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                                                 33.957
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                                                 34.598
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             1287
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                                        79.282
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             1288
                   CB
                       ALA B 227
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                                                         -1.268
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                                                                               6
     ATOM
             1289
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                       ALA B 227
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                       ALA B 227
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                                                36.529
                                                         -1.440
                                                                  1.00 20.00
                                                                               8
25
     ATOM
             1291
                   N
                       LYS B 228
                                        78.467
                                                 36.046
                                                          0.586
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             1292
                       LYS B 228
                                        77.670
     ATOM
                   CA
                                                 37.051
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             1293
                   CB
                       LYS B 228
                                                36.384
                                                          2.179
                                                                  1.00 20.00
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     ATOM
             1294
                   CG
                       LYS B 228
                                        75.705
                                                37.357
                                                          2.890
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                                                                               6
     ATOM
             1295
                       LYS B 228
                                        74.795
                                                                  1.00 20.00
                   CD
                                                38.072
                                                          1.893
                                                                               6
30
             1296
     MOTA
                   CE
                       LYS B 228
                                        73.849 39.049
                                                          2.587
                                                                  1.00 20.00
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            1297
                       LYS B 228
     MOTA
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                                        73.000
                                                39.781
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                                                                  1.00 20.00
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     MOTA
             1299
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                                        79.355
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                                                          2.940
                                                                  1.00 20.00
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     ATOM
             1300
                   N
                       VAL B 229
                                        78.603
                                                39.206
                                                          1.881
                                                                  1.00 20.00
                                                                               7
35
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            1301
                       VAL B 229
                                        79.463
                   CA
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                                                          2.626
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                                                                               6
     ATOM
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                   CB
                       VAL B 229
                                        79.976
                                                41.256
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                                                          1.734
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                                                42.191
     ATOM
            1303
                   CG1 VAL B 229
                                        80.853
                                                          2.540
                                                                  1.00 20.00
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     ATOM
            1304
                   CG2
                       VAL B 229
                                       80.746
                                                          0.561
                                                                  1.00 20.00
                                                40.686
                                                                               6
            1305
                       VAL B 229
                                       78.687
                                                                  1.00 20.00
     ATOM
                   С
                                                40.710
                                                          3.793
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40
                       VAL B 229
    ATOM
            1306
                   0
                                       77.798
                                                41.537
                                                          3.599
                                                                  1.00 20.00
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    ATOM
            1307
                       LEU B 230
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                                                40.284
                   N
                                                                  1.00 20.00
                                                          5.003
                                                                               7
     ATOM
            1308
                   CA
                       LEU B 230
                                       78.370
                                                40.752
                                                          6.213
                                                                  1.00 20.00
                                                                               6
     ATOM
            1309
                   CB
                       LEU B 230
                                       78.740
                                                39.856
                                                          7.395
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                                                                               6
                                       78.276
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	ATOM	1386	CA	ALA	В	246		72.229				
	MOTA	1387				246		71.266				_
	ATOM	1388				246		72.936	19.789	-0.941		-
5	ATOM	1389		ALA	В	246		72.611	19.894	0.239		
	MOTA	1390		GLN	В	247		73.902	18.973			
	ATOM	1391	CA	GLN		247		74.580	18.121	-0.371		
	ATOM	1392	CB	GLN		247		75.535				
	ATOM	1393		GLN	В	247		75.110	16.823	-2.520		
10	MOTA	1394		GLN		247	•	75.139	15.336	-2.811		
	ATOM	1395				247		75.963	14.602	-2.270		
	ATOM	1396		2 GLN	В	247		74.246				
	ATOM	1397	С	GLN				75.343	18.873	0.720	1.00 20.00	
	ATOM	1398	0	GLN	В	247		75.631	18.306	1.773	1.00 20.00	
15	ATOM	1399	N	TYR	В	248		75.648	20.147	0.484	1.00 20.00	
	MOTA	1400	CA	TYR				76.405	20.941	1.454	1.00 20.00	
	MOTA	1401	CB	TYR				77.642	21.531	0.767	1.00 20.00	
	MOTA	1402	CG	TYR	В	248		78.447	20.471	0.052	1.00 20.00	
	ATOM	1403		TYR				79.329	19.648		1.00 20.00	
20	ATOM	1404	CE1	TYR	В	248		79.979	18.589	0.115	1.00 20.00	
	ATOM	1405		TYR				78.243	20.220	-1.306	1.00 20.00	
	MOTA	1406		TYR		248		78.884	19.167	-1.951	1.00 20.00	
	ATOM	1407	CZ	TYR	В	248		79.748	18.352	-1.232	1.00 20.00	
	MOTA	1408	OH	TYR	B	248		80.348	17.280	-1.852	1.00 20.00	
25	MOTA	1409	С	TYR	B :	248		75.596	22.055	2.118	1.00 20.00	
	ATOM	1410	0	TYR				76.132	22.824	2.917	1.00 20.00	
	ATOM	1411	N	VAL	в :	249		74.309	22.135	1.798	1.00 20.00	
	ATOM	1412	CA	VAL				73.452	23.162	2.376	1.00 20.00	
	ATOM	1413	CB	VAL				72.071	23.174	1.695	1.00 20.00	
30	MOTA	1414		VAL				71.117	24.100	2.442	1.00 20.00	6
	MOTA	1415		VAL				72.225	23.632	0.264	1.00 20.00	6
	ATOM	1416	С	VAL				73.262	22.964	3.875	1.00 20.00	6
	ATOM	1417	0	VAL				73.027	21.847	4.341	1.00 20.00	8
	ATOM	1418	N	SER				73.373	24.055	4.628	1.00 20.00	7
35	MOTA	1419	CA	SER				73.206	24.008	6.076	1.00 20.00	6
	ATOM		, CB	SER				73.921	25.198	6.738	1.00 20.00	6
	ATOM	1421	OG	SER				73.428	26.440	6.257	1.00 20.00	8
	ATOM	1422	C	SER				71.717	24.049	6.405	1.00, 20.00	6
40	ATOM	1423	0	SER				70.920	24.577	5.636	1.00 20.00	8
40	ATOM	1424	N	PRO :				71.322	23.479	7.550	1.00 20.00	7
	ATOM	1425	CD	PRO 1				72.130	22.770	8.558	1.00 20.00	6
	ATOM	1426		PRO I				69.905	23.484	7.925	1.00 20.00	6
	ATOM	1427	CB	PRO 1				69.892	22.714	9.252	1.00 20.00	6
45	ATOM	1428	CG	PRO I				71.290	22.936	9.801	1.00 20.00	6
43	ATOM	1429	C	PRO I				69.265	24.870	8.032	1.00 20.00	6
	ATOM	1430	0	PRO I				68.093	25.036	7.688	1.00 20.00	8
	ATOM	1431	N	GLU I				70.017	25.867	8.492	1.00.20.00	7
	ATOM	1432	CA	GLU I				69.462	27.216	8.625	1.00 20.00	6
50	ATOM	1433	CB	GLU E				70.503	28.193	9.196	1.00 20.00	6
50	ATOM	1434	CG	GLU I				71.838	28.180	8.477	1.00 20.00	6
	ATOM	1435	CD	GLU E				72.844	27.257	9.139	1.00 20.00	6
	ATOM	1436	OEI	GLU E	3 2	52		72.429	26.207		1.00 20.00	8
	ATOM	1437		GLU E				74.053	27.581	9.118	1.00 20.00	8
55	ATOM	1438	C	GLU E				68.928	27.744	7.292	1.00 20.00	6
J	ATOM	1439	0	GLU E				67.927	28.459	7.261	1.00 20.00	8
	ATOM	1440	N	LEU E				69.584	27.395	6.189	1.00 20.00	7.
	ATOM	1441	CA	LEU E				69.117	27.850	4.883	1.00 20.00	6
	ATOM	1442	CB	LEU E				70.140	27.527	3.794	1.00 20.00	6
	ATOM	1443	CG	LEU B	2	53		71.127	28.635	3.421	1.00 20.00	6

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	ATOM	1444			B 253		72.121	28.851	4.547	1.00 20.00	6
	MOTA	1445	CD2		B 253		71.858	28.250	2.140	1.00 20.00	6
•	MOTA	1446	-	LEU	B 253		67.774	27.227	4.496	1.00 20.00	6
	ATOM	1447		LEU	B 253		66.997	27.826	3.751	1.00 20.00	8
5	ATOM	1448	N	LEU	B 254		67.506	26.029	5.002	1.00 20.00	7
	ATOM	1449	CA	LEU	B 254		66.271	25.316	4.689		6
	ATOM	1450	CB	LEU	B 254		66.539	23.809	4.689		6
	MOTA	1451	CG	LEU	B 254		67.647	23.322	3.746		6
	ATOM	1452	CDI	L LEU	B 254		67.983	21.873	4.057		6
10	ATOM	1453	CD2	LEU	B 254		67.204	23.475	2.302	1.00 20.00	6
	ATOM	1454	С	LEU	B 254		65.135	25.626	5.662	1.00 20.00	6
	ATOM	1455	0	LEU	B 254		63.959	25.524	5.312	1.00 20.00	8
	ATOM	1456	N		B 255		65.483	26.010	6.883	1.00 20.00	7
	ATOM	1457	CA		B 255		64.472	26.308	7.884	1.00 20.00	6
15	ATOM	1458	СВ		B 255		64.876	25.747	9.252	1.00 20.00	6
	ATOM	1459			B 255		66.154	26.277	9.619	1.00 20.00	8
	ATOM	1460			B 255		64.958	24.230	9.202	1.00 20.00	6
	ATOM	1461	C		B 255		64.205	27.795	8.035	1.00 20.00	
	ATOM	1462	Ö		B 255		63.072	28.241	7.897	1.00 20.00	6 8
20	ATOM	1463	N		B 256		65.250	28.560	8.314	1.00 20.00	7
	ATOM	1464	CA		B 256		65.115	30.001	8.507	1.00 20.00	6
	ATOM	1465	СВ		B 256		66.015	30.444	9.659	1.00 20.00	6
	ATOM	1466	CG		B 256		65.634	29.818	10.987	1.00 20.00	
	ATOM	1467	CD		B 256		66.736	29.922	12.018	1.00 20.00	6 6
25	ATOM	1468		GLU			67.249	31.041	12.232	1.00 20.00	8
	ATOM	1469		GLU			67.086	28.884	12.619	1.00 20.00	8
	ATOM	1470	C		B 256		65.439	30.815	7.262	1.00 20.00	6
	ATOM	1471	Ö		B 256		65.268	32.034	7.252	1.00 20.00	8
	MOTA	1472	N		B 257		65.906	30.141	6.215	1.00 20.00	7
30	ATOM	1473	CA		B 257		66.260	30.814	4.970	1.00 20.00	6
	ATOM	1474	СВ		B 257		65.015	31.458	4.352	1.00 20.00	6
	ATOM	1475	CG		B 257		65.184	31.918	2.915	1.00 20.00	6
	MOTA	1476	CD		B 257		63.885	32.497	2.378	1.00 20.00	6
	ATOM	1477	CE		B 257		63.994	32.841	0.902	1.00 20.00	6
35	ATOM	1478	NZ	LYS !	B 257		65.060	33.847	0.640	1.00 20.00	7
	ATOM	1479	С	LYS I	B 257		67.309	31.885	5.263	1.00 20.00	6
	ATOM	1480	0		B 257		67.270	32.977	4.702	1.00 20.00	8
	ATOM	1481	N	SER I	B 258		68.243	31.563	6.152	1.00 20.00	7
	MOTA	1482	CA	SER I	B 258		69.300	32.494	6.527	1.00 20.00	6
40	ATOM	1483	CB		B 258		69.043	33.028	7.937	1.00 20.00	.6
	MOTA	1484	OG	SER I	B 258		68.893	31.962	8.859	1.00 20.00	8
	ATOM	1485	С	SER I	3 258		70.675	31.829	6.467	1.00 20.00	6
	ATOM	1486	0	SER I	3 258		70.786	30.602	6.542	1.00 20.00	8
	ATOM	1487	N	ALA I	3 259		71.718	32.641	6.329	1.00 20.00	7
45	ATOM	1488	CA	ALA E	3 259		73.081	32.130	6.252	1.00 20.00	6
	ATOM	1489	CB.	ALA E			73.549	32.121	4.809	1.00 20.00	6
	ATOM .	1490	С	ALA E			74.031	32.966	7.102	1.00 20.00	6
	ATOM	1491	0	ALA E			73.882	34.185	7.211	1.00 20.00	8 .
	ATOM	1492	N	CYS E			75.008	32.298	7.704	1.00 20.00	7
50	ATOM	1493	CA	CYS E			75.993	32.960	8.550	1.00 20.00	6
	ATOM	1494	СВ	CYS E			75.574	32.865	10.017	1.00 20.00	6
	ATOM	1495	SG	CYS E			75.303	31.165	10.594		16
	MOTA	1496	C	CYS E			77.328	32.265	8.349	1.00 20.00	6
	ATOM	1497	0	CYS E			77.410	31.280	7.620	1.00 20.00	8
55	ATOM	1498	N	LYS E		•	78.371	32.775	8.993	1.00 20.00	7
	ATOM	1499	CA	LYS B			79.691	32.174	8.869	1.00 20.00	6
	ATOM	1500	CB	LYS B			80.676	32.851	9.821	1.00 20.00	6
	ATOM	1501	CG	LYS B			80.985	34.296	9.472	1.00 20.00	6
	ATOM	1502	CD	LYS B			81.961	34.878	10.475	1.00 20.00	
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	MOTA	1503	CE	LYS	В	261	82.157	36.365	10.259	1.00	20.00	6
	ATOM	1504	NZ	LYS	В	261	83.085	36.922	11.278	1.00	20.00	7
	MOTA	1505	С	LYS	В	261	79.632	30.687	9.187	1.00	20.00	6
	ATOM	1506	0	LYS	В	261	80.258	29.877	8.512	1.00	20.00	8
5	ATOM	1507	N	SER	В	262	78.860	30.346	10.214	1.00	20.00	7
	MOTA	1508	CA	SER	В	262	78.716	28.966	10.659	1.00	20.00	6
	ATOM	1509	CB			262	77.806	28.913	11.895		20.00	6
	ATOM	1510	OG	SER	В	262	77.884	27.657	12.546		20.00	8
	ATOM	1511	C			262	78.161	28.070	9.549		20.00	6
10	ATOM	15ĺ2	Ō			262	78.350	26.856	9.575		20.00	8
	ATOM	1513	N	SER		263	77.466	28.660	8.581		20.00	7
	ATOM	1514	CA	SER		263	76.938	27.870	7.472		20.00	6
	ATOM	1515	CB			263	76.132	28.750	6.507		20.00	
	ATOM	1516	OG			263	75.011		7.156		20.00	8
15	ATOM	1517	C	SER		263	78.123	27.244	6.737		20.00	6
13	ATOM	1518	Ö			263	78.038	26.108	6.273		20.00	8
	ATOM	1519	И	ASP			79.234	27.977	6.642		20.00	7
				ASP		264	80.419	27.448				6
	ATOM	1520	CA						5.961		20.00	
20	MOTA	1521	CB ·			264	81.478	28.538	5.745		20.00	6
20	ATOM	1522	CG			264	81.091	29.539	4.673		20.00	6.
	ATOM	1523		ASP		264	80.286	29.187	3.786		20.00	8
	ATOM	1524		ASP		264	81.617	30.676	4.704		20.00	8
	ATOM	1525	C	ASP		264	81.043	26.312	6.771		20.00	6
~ ~	ATOM	1526	0	ASP		264	81.586	25.365	6.201		20.00	8
25	ATOM	1527	N	LEU		265	80.971	26.415	8.099		20.00	7
	ATOM	1528	CA	LEU		265	81.532	25.390	8.974		20.00	6
	ATOM	1529	CB	LEU		265	81.491	25.848	10.438		20.00	6
	ATOM	1530	CG	LEU		265	82.419	27.035	10.746		20.00	6
	ATOM	1531	CD1	LEU		265	82.204	27.532	12.177		20.00	6
30	ATOM	1532		LEU		265	83.864	26.608	10.541		20.00	6
	ATOM		. C	LEU		265	80.750	24.094	8.800		20.00	6
	ATOM	1534	0	LEU		265	81.306	23.004	8.910		20.00	8
	MOTA	1535	И	TRP		266	79.454	24.208	8.530		20.00	7
	ATOM	1536	CA	TRP		266	78.646	23.017	8.309		20.00	6
35	ATOM	1537	CB	TRP		266	77.167	23.384	8.148		20.00	6 .
	ATOM	1538	CG	TRP		266	76.310	22.245	7.646		20.00	6
	ATOM	1539	CD2	TRP		266	75.455	21.399	8.426		20.00	6
	ATOM	1540	CE2	TRP		266	74.881	20.455	7.542		20.00	6
	ATOM	1541	CE3	TRP		266	75.117		9.785		20.00	6
40	MOTA	1542	CD1	TRP		266	76.220	21.792	6.356		20.00	6
	ATOM	1543	NE1	TRP		266	75.365	20.719	6.288		20.00	7
	ATOM	1544	CZ2	TRP		266	73.988	19.466	7.975		20.00	6
	ATOM	1545	CZ3	TRP			74.227	20.359	10.216		20.00	.6
	ATOM	1546	CH2	TRP		266.	73.674	19.434	9.310		20.00	6
45	ATOM	1547	С	TRP			79.169	22.356	7.038		20.00	6
	ATOM	1548	0	TRP	В	266	79.356	21.142	6.988		20.00	8
	ATOM	1549	N	ALA	В	267	79.411	23.164	6.011	1.00	20.00	7
	ATOM	1550	CA	ALA	В	267	79.930	22.646	4.751		20.00	6
	ATOM	1551	CB	ALA	В	267	80.089	23.772	3.746	1.00	20.00	6
50	ATOM	1552	С	ALA	В	267	81.277	21.976	5.016	1.00	20.00	6
	MOTA	1553	0	ALA			81.570	20.914	4.471	1.00	20.00	8
	ATOM	1554	N	LEU	В	268	82.091	22.596	5.864	1.00	20.00	7
	ATOM	1555	CA	LEU	В	268	83.393	22.030	6.209	1.00	20.00	6
	MOTA	1556	СВ	LEU			84.092	22.898	7.264		20.00	6.
55	ATOM	1557	CG	LEU			85.379	22.332	7.879	1.00	20.00	6
	ATOM	1558		LEU			86.442	22.192	6.803		20.00	6
	ATOM	1559		LEU			85.872	23.263	9.006		20.00	6
	ATOM	1560	C .	LEU			83.193	20.617	6.753		20.00	6
	ATOM	1561	Ö	LEU			83.903	19.684	6.372		20.00	8
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		1560	27	CT W	_	260		00 000	20 463	7 645	1 00	20 00	7
	MOTA	1562	N	GLY				82.220	20.463	7.645		20.00	7
	ATOM	1563	CA	GLY				81.947	19.156	8.217		20.00	6
	MOTA	1564	С	GLY				81.597	18.125	7.156		20.00	6
	ATOM	1565	0	GLY	В	269		82.025	16.971	7.239	1.00	20.00	8
5	MOTA	1566	N	CYS	В	270		80.819	18.530	6.155	1.00	20.00	7
	MOTA	1567	CA	CYS	В	270		80.445	17.613	5.083	1.00	20.00	6
	ATOM	1568	СВ	CYS	-			79.413	18.255	4.148		20.00	6
	ATOM	1569	SG	CYS				77.824	18.654	4.905		20.00	
				CYS				81.682	17.241	4.265		20.00	6
	ATOM	1570	C										
10	ATOM	1571	0	CYS				81.852	16.090	3.866		20.00	8
	MOTA	1572	N	ILE				82.541	18.226	4.012		20.00	
	MOTA	1573	CA	ILE	В	271		83.751	18.000	3.229	1.00	20.00	6
	ATOM	1574	CB	ILE	В	271		84.436	19.339	2.903	1.00	20.00	6
	MOTA	1575	CG2	ILE	В	271		85.784	19.098	2.227	1.00	20.00	6
15	ATOM	1576		ILE				83.508	20.171	2.007	1.00	20.00	6
1,7	ATOM	1577		ILE				83.962	21.607	1.815		20.00	6
				ILE				84.729	17.063	3.934		20.00	6
	MOTA	1578	C										8
	MOTA	1579	0	ILE				85.300	16.174	3.304		20.00	
	MOTA	1580	N	ILE				84.927	17.258	5.236		20.00	-
20	MOTA	1581	CA	ILE	В	272		85.820	16.382	5.987		20.00	6
	MOTA	1582	CB	ILE	В	272		85.902	16.790	7.471	1.00	20.00	6
	ATOM	1583	CG2	ILE	В	272		86.623	15.703	8.277	1.00	20.00	6
	ATOM	1584	CG1	ILE	В	272		86.646	18.120	7.606	1.00	20.00	6
	ATOM	1585		ILE				86.553	18.723	9.011	1.00	20.00	6
25		1586	C	ILE				85.274	14.957	5.901		20.00	6
25	ATOM			ILE					14.003	5.679		20.00	8
	MOTA	1587	0					86.021					7
	MOTA	1588	N	TYR				83.964	14.822	6.072		20.00	
	ATOM	1589	CA	TYR				83.324	13.518	6.006		20:00	6
	ATOM	1590	CB	TYR			-	81.825	13.651	6.287		20.00	6
30	MOTA	. 1591	CG	TYR	В	273		81.064	12.340	6.250	1.00	20.00	6
	ATOM	1592	CD1	TYR	В	273		80.806	11.690	5.041	1.00	20.00	6
	ATOM	1593	CE1	TYR	В	273		80.107	10.486	5.005	1.00	20.00	6
	ATOM	1594	CD2					80.601	11.750	7.427	1.00	20.00	6
	ATOM	1595		TYR				79.904	10.548	7.405	1.00	20.00	6
35	ATOM	1596	CZ			273		79.659	9.922	6.192		20.00	6
33				TYR				78.971	8.736	6.174		20.00	8
	ATOM	1597	OH									20.00	6
	MOTA	1598	C			273		83.550	12.897	4.632			
	ATOM	1599	0	TYR				83.865	11.713	4.526		20.00	8
	ATOM	1600	N	GLN				83.402	13.705	3.586		20.00	7
40	ATOM	1601	CA	GLN	В	274		83.579	13.230	2.220		20.00	6
	ATOM	1602	CB	GLN	В	274		83.176	14.322	1.222	1.00	20.00	6
	ATOM	1603	CG	GLN	В	274		83.149	13.857	-0.230	1.00	20.00	6
	ATOM	1604	CD	GLN	В	274		82.558	14.898	-1.169	1.00	20.00	6
	ATOM	1605		GLN	В	274		82.108	15.961	-0.736	1.00	20.00	8
45	ATOM	1606		GLN				82.548		-2.462		20.00	7
43				GLN				85.013	12.788	1.953	1 00	20.00	6
	ATOM	1607	C				•						. 8
	MOTA	1608	0	GLN				85.239	11.818	1.233		20.00	
	ATOM	1609	N	LEU				85.981	13.498	2.528		20.00	7
•	ATOM	1610	CA	LEU				87.389	13.143	2.333		20.00	
50	ATOM	1611	CB	LEU	В	275		88.311	14.194	2.971		20.00	6
	ATOM	1612	CG	LEU	В	275		88.418	15.561	2.284	1.00	20.00	6
	ATOM	1613	CD1	LEU	В	275		89.325	16.481	3.088	1.00	20.00	6
	ATOM	1614		LEU				88.969	15.379	0.879	1.00	20.00	6
	ATOM	1615	C			275		87.697	11.779	2.940		20.00	6
55				LEU				88.430	10.981	2.354		20.00	8
55	ATOM .	1616	0						11.519	4.112		20.00	7
	ATOM	1617	N	VAL				87.125				20.00	6
	MOTA	1618	CA	VAL				87.353	10.269	4.827			
	MOTA	1619	СВ			276		87.096	10.451	6.342		20.00	6
	ATOM	1620	CG1	VAL	В	276		87.376	9.148	7.082	1.00	20.00	6

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	ATOM	1621		VAL				87.973	11.580	6.891	1.00 20.00	6 6
	ATOM	1622	C	VAL				86.504	9.089	4.336	1.00 20.00	
	ATOM	1623	0	VAL				87.005	7.973	4.195	1.00 20.00	8
	ATOM	1624	N	ALA				85.222	9.337	4.090	1.00 20.00	7
5	MOTA	1625	CA	ALA				84.310	8.291	3.643	1.00 20.00	6
	MOTA	1626	CB	ALA				82.898	8.597	4.124	1.00 20.00	6
	ATOM	1627	C	ALA				84.315	8.115	2.130	1.00 20.00	6
	MOTA	1628	0	ALA	В	277		84.036	7.029	1.627	1.00 20.00	8
	MOTA	1629	N	GLY	В	278		84.632	9.180	1.405	1.00 20.00	7
10	ATOM	1630	CA	GLY	В	278		84.653	9.099	-0.041	1.00 20.00	6
	ATOM	1631	C	GLY	В	278		83.365	9.627	-0.644	1.00 20.00	6
	ATOM	1632	0	GLY	В	278		83.272	9.817	-1.860	1.00 20.00	8
	ATOM	1633	N	LEU	В	279		82.375	9.867	0.211	1.00 20.00	7
	ATOM	1634	CA	LEU	В	279		81.075	10.382	-0.219	1.00 20.00	6
15	ATOM	1635	СВ	LEU	В	279		80.070	9.232	-0.375	1.00 20.00	6
10	ATOM	1636	CG	LEU				80.342	8.114	-1.385	1.00 20.00	6
	ATOM	1637		LEU				79.311	7.009	-1.191	1.00 20.00	6
	ATOM	1638		LEU				80.291	8.660	-2.804	1.00 20.00	6
	ATOM	1639	C	LEU				80.522	11.369	0.812	1.00 20.00	6
20		1640	o	LEU				80.750	11.218	2.007	1.00 20.00	8
·20	ATOM	1641	И	PRO				79.787	12.395	0.361	1.00 20.00	7
	ATOM	1642	CD	PRO				79.403	12.730	-1.020	1.00 20.00	6
	ATOM		CA	PRO				79.230	13.361	1.314	1.00 20.00	6
	MOTA	1643		PRO				78.569	14.397	0.407	1.00 20.00	6
05	MOTA	1644	CB						13.598	-0.802	1.00 20.00	6
25	MOTA	1645	CG	PRO				78.191		2.262	1.00 20.00	6
	ATOM	1646	C			280		78.242	12.662 11.633	1.913	1.00 20.00	8
	MOTA	1647	0	PRO				77.666		3.470	1.00 20.00	7
	MOTA	1648	N	PRO				78.035	13.220		1.00 20.00	6
	MOTA	1649	CD	PRO				78.571	14.535	3.859		6
30	ATOM	1650	CA	PRO				77.145	12.701	4.520	1.00 20.00	6
	ATOM	1651	CB	PRO				77.262	13.746	5.634	1.00 20.00	6
	ATOM	1652	CG			281		78.546	14.450	5.344	1.00 20.00	6
	MOTA	1653	С			281		75.679	12.485	4.142	1.00 20.00	
	ATOM	1654	0	PRO				75.094	11.441	4.442	1.00 20.00	8
· 35	MOTA	1655	N			282		75.088	13.487	3.504	1.00 20.00	7
	ATOM	1656	CA			282		.73.686	13.427	3.123	1.00 20.00	6
		. 1657	СВ			282		73.006	14.734	3.531	1.00 20.00	6
	ATOM	1658	CG			282		73.300	15.146	. 4.947	1.00 20.00	
	ATOM	1659		PHE				72.624	14.560	6.013	1.00 20.00	6
40 /	ATOM	1660		PHE				74.295	16.085	5.218	1.00 20.00	6
	ATOM	1661		PHE				72.934	14.902	7.331	1.00 20.00	6
	ATOM	1662		PHE				74.613	16.433	6.530	1.00 20.00	6
	ATOM	1663	CZ			282		73.930	15.840	7.591	1.00 20.00	6
	ATOM	1664	С			282		73.527	13.191	1.628	1.00 20.00	6
45	ATOM	1665	0			282		73.797			1.00 20.00	8
	ATOM	1666	N			283		73.080	11.994	1.267	1.00 20.00	7
	ATOM	1667	CA			283		72.888	11.635	-0.134	1.00 20.00	6
	ATOM	1668	CB	ARG	В	283		73.931	10.598	-0.559	1.00 20.00	6
	ATOM	1669	CG	ARG	В	283	-	75.358	10.928	-0.151	1.00 20.00	6
50	ATOM	1670	CD	ARG	В	283		76.326	9.883	-0.687	1.00 20.00	6
	ATOM	1671	NE	ARG	В	283		76.054	8.555	-0.142	1.00 20.00	7
•	ATOM	1672	CZ			283		76.404	8.159	1.077	1.00 20.00	6
	ATOM	1673		ARG				77.047	8.986	1.893	1.00 20.00	7
	ATOM	1674				283 .		76.108	6.933	1.484	1.00 20.00	7
55	ATOM	1675	C			283		71.493	11.046	-0.331	1.00 20.00	6
	ATOM	1676	0.			283		70.957	10.391	0.563	1.00 20.00	8
	ATOM	1677	N			284		70.911	11.276	-1.502	1.00 20.00	7
	ATOM	1678	CA			284		69.579	10.755	-1.796	1.00 20.00	6
	ATOM	1679	CB			284		68.532	11.484	-0.961	1.00 20.00	6
	VIOL	1013	CD	*****		231		55.555				

	ATOM .	1680	С	ALA	В	284	69.278	10.921	-3.273	1.00 20.00	6
	ATOM	1681	0	ALA	В	284	70.007	11.611	-3.984	1.00 20.00	8
	ATOM	1682	N	GLY	В	285	68.191	10.299	-3.722	1.00 20.00	7
	ATOM	1683	CA	GLY	В	285	67.807	10.360	-5.122	1.00 20.00	
5	ATOM	1684	С			285	67.561	11.737	-5.707	1.00 20.00	
_	ATOM	1685	Ö			285	67.775	11.955	-6.899	1.00 20.00	
	ATOM	1686	N			286	67.089	12.673	-4.892	1.00 20.00	
	ATOM	1687	CA			286	66.835	14.018	-5.386	1.00 20.00	
	ATOM	1688	CB			286	65.403	14.137	-5.930		
10		1689	CG			286				1.00 20.00	
10	ATOM						64.342	13.825	-4.885	1.00 20.00	
	ATOM	1690		ASN			64.292	14.450	-3.826	1.00 20.00	8
	ATOM	1691		ASN			63.477		-5.190	1.00 20.00	7
	ATOM	1692	C			286	67.076	15.042	-4.291	1.00 20.00	
	ATOM	1693	0			286	67.368	14.682	-3.152	1.00 20.00	8
15	ATOM	1694	N	GLU			66.955	16.317	-4.636	1.00 20.00	7
	ATOM	1695	CA	GLU			67.185	17.377	-3.669	1.00 20.00	6
	ATOM	1696	CB	GLU			67.181	18.738	-4.365	1.00 20.00	6
	MOTA	1697	CG	GLU	В	287	68.537	19.095	-4.944	1.00 20.00	. 6
	MOTA	1698	CD	GLU	В	287	68.524	20.385	-5.735	1.00 20.00	6
20	MOTA	1699		GLU			67.911	21.371	-5.267	1.00 20.00	8
	ATOM -	1700	OE2	GLU	В	287	69.144	20.410	-6.823	1.00 20.00	8
	ATOM	1701	С	GLU	В	287	66.225	17.394	-2.492	1.00 20.00	6
	MOTA	1702	0	GLU	В	287	66.658	17.554	-1.354	1.00 20.00	8
	ATOM	1703	Ń	TYR	В	288	64.932	17.233	-2.753	1.00 20.00	7
25	ATOM	1704	CA	TYR	В	288	63.955	17.239	-1.670	1.00 20.00	6
	ATOM	1705	CB	TYR			62.553	16.899	-2.184	1.00 20.00	6
	ATOM	1706	CG	TYR			61.530	16.780	-1.070	1.00 20.00	6
	ATOM	1707		TYR			60.984	17.917	-0.470	1.00 20.00	6
	ATOM	1708		TYR			60.090	17.814	0.600	1.00 20.00	6
30	ATOM	1709		TYR			61.154	15.529	-0.573	1.00 20.00	6
20	ATOM	1710	CE2	TYR			60.265	15.414	0.498	1.00 20.00	6
	ATOM	1711	CZ	TYR			59.740	16.561	1.078	1.00 20.00	6
	ATOM	1712	OH	TYR			58.884	16.454	2.149	1.00 20.00	8
	ATOM	1713	C	TYR			64.337	16.238	-0.587	1.00 20.00	6
35	ATOM	1714	0	TYR			64.254	16.545	0.598	1.00 20.00	8
))	ATOM	1715	N	LEU			64.750		-1.001		7
		1716						15.041	•	1.00 20.00	
	ATOM		CA	LEU			65.137	13.989	-0.064	1.00 20.00	6
	ATOM	1717	CB	LEU			65.283	12.649	-0.797	1.00 20.00	6
40	ATOM	1718	CG	ĻEU			63.984	11.985	-1.274	1.00 20.00	6
40	ATOM	1719		LEU			64.314	10.802	-2.179	1.00 20.00	6
	MOTA	1720		LEU			63.160	11.530	-0.068	1.00 20.00	6
	ATOM	1721	С	LEU			66.431	14.310	0.685	1.00 20.00	6
	ATOM	1722	0	LEU			66.604	13.914	1.840	1.00 20.00	8
4 ==	ATOM	1723	N	ILE			67.340	15.017	0.025	1.00 20.00	7
45	MOTA	1724		ILE						1.00 20.00	6
	MOTĄ	1725	CB	ILE			69.583	15.985	-0.366	1.00 20.00	6
	MOTA	1726		ILE			70.778	16.609	0.359	1.00 20.00	6
	ATOM	1727		ILE			70.046	14.887	-1.330	1.00 20.00	6
	ATOM	1728		ILE	В	290	70.844	15.398	-2.518	1.00 20.00	6
50	ATOM	1729	C .	ILE	В	290	68.307	16.424	1.743	1.00 20.00	6
	ATOM	1730	0	ILE	В	290	68.807	16.317	2.862	1.00 20.00	8
	ATOM	1731	N	PHE			67.491	17.420	1.411	1.00 20.00	7
	ATOM	1732	CA	PHE	В	291	67.143	18.462	2.372	1.00 20.00	6
	ATOM	1733	CB	PHE			66.222	19.502	1.731	1.00 20.00	6
55	ATOM	1734	CG	PHE			66.869	20.289	0.628	1.00 20.00	6
	ATOM	1735		PHE			68.255	20.420	0.568	1.00 20.00	6
	ATOM	1736		PHE			66.094	20.931	-0.332	1.00 20.00	6
	ATOM	1737		PHE			68.859	21.182	-0.435	1.00 20.00	6
	ATOM	1738		PHE			66.690	21.697	-1.340	1.00 20.00	6

	ATOM	1739	CZ	חווס	R	2,91		68.074	21.822	-1.390	1.00 20.00	. 6
	ATOM	1740	C			291		66.453	17.848	3.576	1.00 20.00	
	ATOM	1741	Ö			291		66.664	18.262	4.718	1.00 20.00	8
	ATOM	1742	Ŋ		_	292		65.629	16.847	3.303	1.00 20.00	
5		1743						64.887	16.154	4.341	1.00 20.00	
,	ATOM		CA									6
	ATOM	1744 1745	CB	GLN		292		64.006 62.953	15.090	3.687	1.00 20.00	6
	ATOM		CG						14.486	4.572	1.00 20.00	_
	ATOM	1746	CD			292		61.895	13.750	3.763	1.00 20.00	6
10	ATOM	1747		GLN				62.208	12.835	2.997	1.00 20.00	8
10	ATOM	1748		GLN				60.637	14.155	3.924	1.00 20.00	7
	ATOM	1749	C			292		65.865	15.522	5.329	1.00 20.00	6
•	MOTA	1750	0			292		65.689	15.630	6.540	1.00 20.00	8
	MOTA	1751	N			293		66.907	14.875	4.812 5.683	1.00 20.00	7
15	ATOM	1752	CA			293		67.898	14.244		1.00 20.00	6
13	ATOM	1753 1754	CB			293 293		68.850 68.197	13.372	4.865	1.00 20.00	6
	ATOM		CG				•		12.135	4.278	1.00 20.00	6
	ATOM	1755	·CD			293		69.217	11.260	3.554	1.00 20.00	6
	ATOM	1756	CE			293		68.575 69.553	9.972	3.051	1.00 20.00	6
20	ATOM	1757 1758	NZ	LYS		293		68.698	9.099 15.287	2.339	1.00 20.00	7 .
20	ATOM	1759	С	LYS						6.468 7.634	1.00 20.00 1.00 20.00	6
	ATOM ATOM	1760	N O	ILE				69.044 68.989	15.074 16.411	5.827	1.00 20.00	8 7·
	ATOM	1761	CA	ILE			•	69.745	17.480	6.472	1.00 20.00	6
	ATOM	1762	CB			294		70.026	18.632	5.474	1.00 20.00	6
25	ATOM	1763		ILE		294		70.489	19.881	6.223	1.00 20.00	6
23	ATOM	1764		ILE				71.070	18.178	4.443	1.00 20.00	6
	ATOM	1765		ILE				71.266	19.159	3.303	1.00 20.00	6
	MOTA	1766	C	ILE				69.035	18.045	7.712	1.00 20.00	6
	ATOM	1767	Ö	ILE				69.618	18.091	8.798	1.00 20.00	8
30	. ATOM	1768	N			295		67.783		. 7.564	1.00 20.00	7
	ATOM	1769	CA	ILE		295		67.068	19.037	8.707	1.00 20.00	6
	ATOM	1770	CB			295		65.710	19.647	8.300	1.00 20.00	6
	ATOM	1771		ILE				65.927	20.749	7.265	1.00 20.00	6
	ATOM	1772		ILE				64.784	18.559	7.762	1.00 20.00	6
35	ATOM	1773		ILE			•	63.356	19.037	7.558	1.00 20.00	6
	ATOM	1774	С	ILE				66.831	18.045	9.842	1.00 20.00	6
	ATOM	1775	0	ILE				66.540	18.447	10.967	1.00 20:00	8
	ATOM	1776	N	LYS	В	296		66.956	16.753	9.550	1.00 20.00	7
	ATOM	1777	CA	LYS	В	296		66.765	15.724	10.569	1.00 20.00	6
40	ATOM	1778	CB	LYS	В	296		65.907	14,576	10.019	1.00 20.00	6
	ATOM	1779	CG	LYS	В	296		64.535	15.010	9.538	1.00 20.00	6
	ATOM	1780	CD	LYS	В	296		63.739	13.851	8.951	1.00 20.00	6
	ATOM	1781	CE	LYS	В	296		63.296	12.873	10.025	1.00 20.00	6
	ATOM	1782	NZ	LYS	В	296		62.375	11.828	9.482	1.00 20.00	7
45	ATOM	1783	С	LYS	В	296		68.116	15.176	11.018	1.00 20.00	6
	MOTA	1784	0	LYS				68.178	14.261	11.838	1.00 20.00	8
	MOTA	1785	N	LEU				69.190	15.746	10.474	1.00 20.00	7
	MOTA	1786	CA	LEU				70.551	15.320	10.791	1.00 20.00	6
	ATOM	1787	CB	LEU				70.911	15.680	12.236	1.00 20.00	6
50	ATOM	1788	CG	LEU				72.398	15.538	12.585	1.00 20.00	6
	ATOM	1789		LEU				73.215	16.555	11.771	1.00 20.00	6
	ATOM	1790		LEU				72.605	15.762	14.076	1.00 20.00	6
	ATOM	1791	C	LEU				70.635	13.810	10.592	1.00 20.00	6
	MOTA	1792	0	LEU				71.150	13.080	11.434	1.00 20.00	8
55	ATOM	1793	N	GLU				70.128	13.351	9.456	1.00 20.00	7
	ATOM	1794	CA	GLU				70.115	11.934	9.148	1.00 20.00	6
	ATOM	1795	CB	GLU				68.817	11.597	8.416	1.00 20.00	6
	ATOM	1796	CG	GLU				68.568	10.123	8.233	1.00 20.00	6
	MOTA	1797	CD	GLU	В	298		67.254	9.858	7.535	1.00 20.00	6

	AȚOM ATOM ATOM	1798 1799 1800		GLU GLU	В	298	66.214 67.261 71.309	10.331 9.185 11.446	8.043 6.484 8.332	1.00	20.00 20.00 20.00	8 8 6
			0				71.309	11.523	7.104			
_	ATOM	1801		GLU							20.00	8
5	ATOM	1802	N	TYR			72.325	10.946	9.027		20.00	7
	MOTA	1803	CA	TYR			73.519	10.405	8.390		20.00	6
	ATOM	1804	CB	TYR			74.444	11.521	7.880		20.00	6
	ATOM	1805	CG			299	75.330	12.130	8.953		20.00	6
_	ATOM	1806		TYR			74.796	12.962	9.935		20.00	6
10	ATOM	1807		TYR			75.589	13.482	10.951		20.00	6
	MOTA	1808		TYR			76.692	11.833	9.013		20.00	6
	ATOM	1809		.TYR			77.499	12.352	10.032		20.00	6
	ATOM	1810	CZ	TYR			76.935	13.173	10.995		20.00	6
	MOTA	1811	ОН			299	77.701	13.687	12.006	1.00	20.00	8
15	ATOM	1812	С	TYR			74.245	9.600	9.456		20.00	6
	ATOM	1813	0	TYR	В	299	73.913	9.688	10.631	1.00	20.00	8
	ATOM	1814	N	ASP	В	300	75.229	8.808	9.052		20.00	. 7
	MOTA	1815	CA	ASP	В	300	75.991	8.030	10.016		20.00	6
	MOTA	1816	CB	ASP	В	300	75.291	6.700	10.304	1.00	20.00	6
20	ATOM	1817	CG	ASP	В	300	74.898	5.968	9.048	1.00	20.00	6
	ATOM	1818	OD1	ASP	В	300	75.806	5.594	8.274	1.00	20.00	8
	ATOM	1819	OD2	ASP	В	300	73.681	5.771	8.832	1.00	20.00	8
	ATOM	1820	С	ASP	B,	300	77.397	7.799	9.488	1.00	20.00	6
	ATOM	1821	0	ASP	В	300	77.651	7.976	8.297	1.00	20.00	8
25	MOTA	1822	.N	PHE	В	301	78.307	7.417	10.378	1.00	20.00	7
	MOTA	1823	CA	PHE	В	301	79.695	7.186	9.996	1.00	20.00	6
	MOTA	1824	CB	PHE	В	301	80.655	7.664	11.093		20.00	6
	ATOM	1825	CG	PHE	В	301	80.488	9.103	11.481		20.00	6
	MOTA	1826		PHE			79.493	9.487	12.370	1.00	20.00	6
30	ATOM	1827		PHE			81.346	10.075	10.970		20.00	6
	MOTA	1828		PHE			79.352	10.823	12.750		20.00	6
	MOTA	1829	CE2	PHE			81.214	11.408	11.342		20.00	6
	MOTA	1830	CZ	PHE			80.215	11.783			20.00	6
	ATOM	1831	С	PHE	В	301	80.009	5.722	9.744		20.00	6
35	ATOM	1832	0	PHE			79.506	4.839	10.442		20.00	8
	ATOM	1833	N	PRO	В	302	80.842	5.440	8.732	1.00	20.00	7
	MOTA	1834	CD	PRO			81.330	6.316	7.654		20.00	6
	MOTA	1835	CA	PRO	В	302	81.191	4.044	8.466	1.00	20.00	6
	MOTA	1836	CB	PRO			81.838	4.105	7.084		20.00	6
40	ATOM	1837	CG	PRO	В	302	82.425	5.479	7.046		20.00	6
	MOTA	1838	С	PRO			82.168	3.629	9.569		20.00	6
	MOTA	1839	0	PRO			82.887	4.469	10.111		20.00	8
	MOTA	1840	N	ALA			82.185	2.345	9.908		20.00	7
	ATOM	1841	CA	ALA			83.052	1.836	10.968		20.00	6
45	ATOM	1842	СВ	ALA			82.993	0.310				6
	ATOM	1843	С	ALA			84.513	2.294	10.939		20.00	6
	ATOM	1844	0	ALA			85.078	2.637	11.979		20.00	8
	MOTA	1845	N	ALA			85.121	2.306	9.756		20.00	7
	ATOM	1846	CA	ALA			86.527	2.684	9.605		20.00	6
50	ATOM	1847	CB	ALA			86.971	2.423	8.165		20.00	6
	ATOM	1848	С	ALA			86.894	4.119	10.001		20.00	6
	ATOM	1849	0	ALA			87.983	4.367	10.520		20.00	8
	ATOM	1850	N	PHE			85.985	5.053	9.742		20.00	7
	ATOM	1851	CA	PHE			86.183	6.473	10.034		20.00	6
. 55	ATOM	1852	CB	PHE			84.822	7.115	10.312		20.00	6
	ATOM	1853	CG	PHE			84.705	8.522	9.815		20.00	6
	ATOM	1854		PHE			85.303	9.572	10.502		20.00	6
	ATOM	1855		PHE			84.003	8.800	8.646		20.00	6
	ATOM	1856	CEI	PHE	В	305	85.202	10.881	10.033	1.00	20.00	6

	ATOM ATOM ATOM	1857 1858 1859	CE2 CZ C	PHE	B B	305 305		83.896 84.496 87.153	10.106 11.147 6.789	8.167 8.862 11.182	1.00 20.00 1.00 20.00 1.00 20.00	6
5	ATOM ATOM	1860 1861	O N	PHE	В	305 306		86.964 88.190	6.342 7.565	12.312 10.883	1.00 20.00 1.00 20.00	
	ATOM	1862	CA			306		89.176	7.945	11.894	1.00 20.00	
	ATOM	1863	CB			306		90.179		11.295	1.00 20.00	
•	ATOM	1864	CG			306		90.695	8.531	9.940	1.00 20.00	6
	ATOM	1865		PHE				91.292	7.284	9.747	1.00 20.00	6
10	ATOM	1866		PHE				90.588	9.395	8.853	1.00 20.00	
	ATOM	1867		PHE				91.774	6.906	8.490	1.00 20.00	6
	ATOM	1868 1869	CEZ	PHE		306		91.067	9.027	7.590	1.00 20.00	6
	ATOM ATOM	1870	C			306		91.662 88.445	7.780 8.575	7.408 13.086	1.00 20.00 1.00 20.00	6 6
15	ATOM	1871	Ö			306		87.731	9.566	12.936	1.00 20.00	8
13	ATOM	1872	N	PRO				88.614	7.995	14.288	1.00 20.00	7
	ATOM	1873	CD	PRO				89.482	6.834	14.555	1.00 20.00	6
	ATOM	1874	CA	PRO				87.983	8.459	15.530	1.00 20.00	6
	ATOM	1875	СВ	PRO				88.748	7.691	16.606	1.00 20.00	6
20	ATOM	1876	CG	PRO				89.018	6.388	15.928	1.00 20.00	6
	MOTA	1877	С	PRO	В	307		87.986	9.965	15.784	1.00 20.00	6
	ATOM	1878	0	PRO	В	307		86.936	10.565	16.025		
	ATOM~	1879	N	LYS				89.162	10.575	15.745	1.00 20.00	7
	ATOM	1880	CA	LYS				89.260	12.004	15.992	1.00 20.00	6
25	MOTA	1881	CB	LYS				90.728		16.149	1.00 20.00	6
	ATOM	1882	CG	LYS				91.338	11.805	17.410	1.00 20.00	6
•	MOTA	1883	CD	LYS				92.806	12.140	17.591	1.00 20.00	6
	ATOM	1884	CE	LYS			•		11.457	18.847	1.00 20.00	6
30	MOTA ATOM	1885 1886	· NZ C	LYS LYS				94.816	11.573	18.985	1.00 20.00	7
30	ATOM	1887	0	LYS				88.572 87.985	12.808 13.855	14.894 15.167	1.00 20.00	6 8
	ATOM	1888	N	ALA				88.629	12.318	13.659	1.00 20.00	7
	ATOM	1889	CA	ALA				87.967	13.011	12.557	1.00 20.00	6
	ATOM	1890	СВ	ALA				88.328	12.369	11.231	1.00 20.00	6
35	MOTA	1891	С	ALA				86.460	12.936	12.787	1.00 20.00	6
	MOTA	1892	0	ALA	В	309		85.735	13.903	12.552	1.00 20.00	8
	MOTA	1893	N	ARG	В	310		85.986	11.780	13.246	1.00 20.00	7
	ATOM	1894	CA	ARG		310		84.561	11.619	13.513	1.00 20.00	. 6
	ATOM	1895	СB	ARG				84.246	10.194	13.979	1.00 20.00	6
40	ATOM	1896	CG	ARG				82.844	10.069	14.561	1.00 20.00	6
	ATOM	1897	CD	ARG		310		82.408	8.632	14.789	1.00 20.00	6
	ATOM ATOM	1898 1899	NE CZ	ARG ARG				81.060	8.593	15.355	1.00 20.00	7
	ATOM	1900		ARG				80.259 80.665	7.532 6.401	15.328 14.759	1.00 20.00 1.00 20.00	6 7
45	ATOM	1901		ARG				79.048			1.00 20.00	7
1.5	ATOM	1902	C	ARG	_			84.110	12.613	14.583	1.00 20.00	6
	ATOM	1903	ō	ARG				83.080	13.274	14.436	1.00 20.00	8
	ATOM	1904	N	ASP				84.876	12.707	15.666	1.00 20.00	7
	ATOM	1905	CA	ASP				84.535	13.629	16.740	1.00 20.00	6
50	ATOM	1906	СВ	ASP				85.574	13.555	17.864	1.00 20.00	6
	MOTA	1907	CG	ASP	В	311		85.260	14.505	19.006	1.00 20.00	6
	ATOM	1908		ASP				85.782	15.636	19.010	1.00 20.00	8
	ATOM	1909	OD2	ASP				84.480	14.124	19.901	1.00 20.00	8
	ATOM	1910	С	ASP				84.445	15.054	16.198	1.00 20.00	6
55	ATOM	1911	0	ASP				83.539	15.800	16.564	1.00 20.00	8
	ATOM	1912	N	LEU				85.371	15.423	15.313	1.00 20.00	7
	ATOM	1913	CA	LEU				85.362	16.769	14.736	1.00 20.00	6
	ATOM ATOM	1914 1915	CB CG	LEU				86.604	16.999	13.869	1.00 20.00	6
	111 OF	1910	CG	LEU	٥	J14		86.662	18.329	13.099	1.00 20.00	6

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ATOM
              1916
                    CD1 LEU B 312
                                         86.424 19.510
                                                          14.037
                                                                   1.00 20.00
                    CD2 LEU B 312
      ATOM
              1917
                                         88.018
                                                 18.450
                                                          12.414
                                                                   1.00 20.00
      ATOM
              1918
                    C
                         LEU B 312
                                         84.112
                                                 17.008
                                                          13.899
                                                                   1.00 20.00
                                                                                6
      MOTA
              1919
                    0
                        LEU B 312
                                         83.456
                                                 18.039
                                                          14.035
                                                                   1.00 20.00
                                                                                8
      ATOM
              1920
                        VAL B 313
                    N
                                         83.786
                                                 16.051
                                                          13.033
                                                                  1.00 20.00
      MOTA
                        VAL B 313
              1921
                    CA
                                         82.611
                                                 16.171
                                                          12.183
                                                                  1.00 20.00
                                                                                6
      ATOM
              1922
                    CB
                        VAL B 313
                                         82.464
                                                 14.942
                                                          11.255
                                                                  1.00 20.00
                                                                                6
      ATOM
              1923
                    CG1
                        VAL B 313
                                         81.121
                                                 14.973
                                                          10.551
                                                                  1.00 20.00
                                                                                6
      ATOM
             1924
                    CG2 VAL B 313
                                         83.595
                                                 14.935
                                                          10.228
                                                                  1.00 20.00
                                                                                6
      ATOM
             1925
                        VAL B 313
                    С
                                        81.354
                                                 16.315
                                                         13.036
                                                                  1.00 20.00
                                                                                6
      ATOM
             1926
                        VAL B 313
                    0
                                        80.467
                                                 17.111
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	ATOM	1977	CA .	ASP B 320		24.687	17.490	1.00 20.00	6
	ATOM	1978		ASP B 320	72.091	26.061	18.129	1.00 20.00	6
5	MOTA	1979		ASP B 320	72.058		17.492	1.00 20.00	8
	MOTA	1980	OD1	ASP B 320	72.506	27.036		1.00 20.00	8
	ATOM	1981	OD2	ASP B 320	71.595	26.166	19.284	1.00 20.00	6
	ATOM	1982		ASP B 320	73.415	25.419	15.492	1.00 20.00	8
	ATOM	1983		ASP B 320	74.496	25.089	15.965		7
10	ATOM	1984	N	ALA B 321	73.294	26.372	14.576	1.00 20.00	6
10	ATOM	1985		ALA B 321	74.450	27.078	14.028	1.00 20.00	
	ATOM	1986		ALA B 321	73.982	28.109	13.006	1.00 20.00	6
	ATOM	1987		ALA B 321	75.359	27747	15.065	1.00 20.00	6
	ATOM	1988		ALA B 321	76.535	27.992	14.790	1.00 20.00	8,
1.5		1989	N	THR B 322	74.829	28.035	16.252	1.00 20.00	7
15	MOTA	1990	CA	THR B 322	75.631	28.681	17.292	1.00 20.00	6
	MOTA		CB	THR B 322	74.755	29.491	18.271	1.00 20.00	6
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	MOTA	1992		THR B 322	73.928	30.527	17.519	1.00 20.00	6
	MOTA	1993		THR B 322	76.437	27.684	18.108	1.00 20.00	6
20	ATOM	1994	С		77.166	28.071	19.019	1.00 20.00	8
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	MOTA	1996	N	LYS B 323	77.048	25.378	18.517	1.00 20.00	6
	MOTA	1997	CA	LYS B 323		24.378	19.155	1.00 20.00	6
	MOTA	1998	CB	LYS B 323	76.080	24.992	20.209	1.00 20.00	6
25	MOTA	1999	CG	LYS B 323	75.180	23.931	20.924	1.00 20.00	6
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	ATOM	2002	NZ	LYS B 323	74.144	25.514	17.664	1.00 20.00	6
•	MOTA	2003	С	LYS B 323	78.066	24.631	18.040	1.00 20.00	8
30	MOTA	2004	0	LYS B 323	78.520	23.557		1.00 20.00	7
	ATOM	2005	N	ARG B 324	78.427	25.195	16.517	1.00 20.00	6
	MOTA	2006	CA	ARG B 324	79.408	24.545	15.656	1.00 20.00	6
	MOTA	2007	CB	ARG B 324	79.108	24.834	14.186	1.00 20.00	6
	ATOM	2008	CG	ARG B 324	77.824	24.177	13.728	1.00 20.00	6
35	ATOM	2009	CD	ARG B 324	77.468	24.505	12.297		7
33	ATOM	2010	NE	ARG B 324	76.060	24.202	12.069	1.00 20.00	6
	MOTA	2011	CZ	ARG B 324	75.277	24.873	11.233	1.00 20.00	7
	ATOM	2012		ARG B 324	75.764	25.888	10.523	1.00 20.00	
	ATOM	2013		ARG B 324	73.992	24.551	11.140	1.00 20.00	7 6
40	ATOM	2014	С	ARG B 324	80.811	25.011	16.008	1.00 20.00	
40	ATOM	2015	Ö	ARG B 324	81.070	26.212	16.131	1.00 20.00	8
	MOTA	2016	N.	LEU B 325	81.711	24.049	16.180	1.00 20.00	
	ATOM	.2017		LEU B 325	83.090	24.350	16.520	1.00 20.00	
	ATOM	2018	CB	LEU B 325	83.913	23.061	16.550	1.00 20.00	
45		2019	CG	LEU B 325	85.274	23.123	17.241	1.00 20.00	
45	MOTA	2020		LEU B 325	85.093		18.682	1.00 20.00	6
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	ATOM			LEU B 325	83.649			1.00 20.00	8
	MOTA	2023		GLY B 326	84.139		15.946	1.00 20.00	
50	ATOM	2024		GLY B 326	84.697			1.00 20.00	
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55	MOTA	2029		CYS B 327	80.233				
	MOTA	2030		CYS B 327	79.534				
	MOTA	2031		CYS B 327					
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	MOTA	2033	3 0	CYS B 327	82.565	30.410	, _,,,,,,		

	ATOM ATOM	2034 2035	N CA	GLU GLU		328 328	81.523 81.714	32.005 33.052	16.178 17.167		20.00	
	ATOM	2036	CB			328	81.087	34.348	16.632	_	20.00	_
_	ATOM	2037	CG			328	81.734	34.772	15.300		20.00	
5	ATOM	2038	CD	GLU		328	80.962	35.842	14.539		20.00	6
	ATOM	2039		GLU			79.738	35.676	14.343		20.00	
	ATOM	2040	OE2				81.588	36.840	14.116		20.00	8
	ATOM	2041	С			328	81.187	32.701	18.560		20.00	6
	ATOM	2042	0	GLU			81.850	32.983	.19.562	1.00	20.00	8
10	ATOM	2043	N			329	80.016	32.073	18.631	1.00	20.00	7
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	ATOM	2046	CG			329	77.028	32.355	19.315		20.00	6
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15	MOTA	2048	OE1	${\tt GLU}$	В	329	77.859	31.910	17.120	1.00	20.00	8
	ATOM	2049	OE2	GLU			76.267	33.413	17.323	1.00	20.00	8
	ATOM	2050	С	GLU	В	329	80.264	30.616	20.605	1.00	20.00	6
	MOTA	2051	0	GLU	В	329	80.182	30.436	21.819	1.00	20.00	8
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20	ATOM	2053	CA	MET	В	330	81.880	28.813	20.354		20.00	6
	ATOM	2054	CB	MET	В	330	81.872	27.600	19.419	1.00	20.00	6
	ATOM	2055	CG	MET	В	330	80.552	26.822	19.436	1.00	20.00	6
	ATOM	2056	SD	MET	В	330	80.117	26.254	21.104	1.00	20.00	16
	MOTA	2057	CE	MET	В	330	81.265	24.895	21.311	1.00	20.00	6
25	ATOM	2058	С	MET	В	330	83.302	29.330	20.547		20.00	6
	ATOM	2059	0	MET			84.236	28.564	20.754		20.00	8
	MOTA	2060	Ν.	GLU			83.443	30.647	20.471		20.00	7
	ATOM	2061	CA	GLU	В	331	84.716	31.338	20.656	1.00	20.00	6
	ATOM	2062	CB	GLU		331	85.357	30.921	21.987		20.00	6
30	ATOM	2063	CG	GLU	В	331	84.371	30.886	23.163	1.00	20.00	6
	ATOM	2064	CD	GLU			83.478	32.127	23.270	1.00	20.00	6
	ATOM	2065		GLU			82.483	32.064	24.021		20.00	8
	ATOM	2066	OE2	GLU			83.759	33.159	22.625		20.00	8
	ATOM	2067	С	GLU			85.742	31.247	19.523		20.00	6
35	ATOM.	2068	0	GLU		331	86.952	31.264	19.761		20.00	8
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40	ATOM	2073	N	TYR			88.002	30.366	15.875		20.00	7
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	ATOM	2075	CB	TYR			89.625	30.053	14.093		20.00	6
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45	ATOM	2078		TYR			87.872				20.00	6
	ATOM	2079		TYR			87.747	31.011	12.686		20.00	6
	ATOM	2080		TYR			86.831	30.923	11.624		20.00	6
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50	ATOM	2083	С	TYR			89.958	28.800.	16.252		20.00	6
	ATOM	2084	0	TYR				27.721	15.971		20.00	8
	ATOM	2085	N	GLY			90.242	29.469	17.369		20.00	7
	ATOM	2086	CA	GLY			91.193	28.921	18.327		20.00	6
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55	ATOM	2088	0	GLY			91.577	26.564	18.558		20.00	8
	ATOM	2089	N	PRO			89.603	27.320	19.309		20.00	7
	ATOM	2090	CD	PRO			88.703	28.372	19.814		20.00	6
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	ATOM	2153	CE2	PHE	В	342	90.843	20.898	12.742	1.00 20.00	6
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	ATOM	2155	С			342	96.077	18.718	15.101	1.00 20.00	6
5	ATOM	2156	ō			342	96.932	19.584	14.902	1.00 20.00	8
•	ATOM	2157	N			343	96.173	17.829	16.083	1.00 20.00	7
	ATOM	2158	CA			343	97.293	17.857	17.022	1.00 20.00	6
	ATOM	2159	CB			343	97.330		17.022	1.00 20.00	
	ATOM	2160	CG			343		16.564			6
10		2161	CD			343	98.475	16.525	18.839	1.00 20.00	6
10	MOTA						98.372	15.365	19.813	1.00 20.00	6
	ATOM	2162		GLU			98.290	14.201	19.359	1.00 20.00	8
	ATOM	2163		GLU			98.379	15.622	21.036		8
	ATOM	2164	С			343	98.683	18.113	16.430	1.00 20.00	6
	MOTA	2165	0			343	99.419	18.969	16.925	1.00 20.00	8
15	ATOM	2166	N			344	99.047	17.382	15.383	1.00 20.00	7
•	ATOM	2167	CA			344	100.370	17.549	14.781	1.00 20.00	6
	MOTA	2168	CB			344.	100.848	16.219	14.192	1.00 20.00	6
	MOTA	2169	OG	SER			100.072	15.856	13.065	1.00 20.00	8
	ATOM	2170	С	SER			100.467	18.629	13.702	1.00 20.00	6
20	ATOM	2171	0	SER	В	344	101.485	18.732	13.025	1.00 20.00	8
	MOTA	2172	N	VAL	В	345	99.423	19.435	13.544	1.00 20.00	7
	MOTA	2173	CA	VAL			99.430	20.486	12.527	1.00 20.00	6
	ATOM	2174	CB	VAL			97.985	20.843	12.075	1.00 20.00	6
	ATOM	2175	CG1	VAL	B	345	98.015	22.042	11.120	1.00 20.00	6
25	ATOM	2176	CG2	VAL	B	345	97.335	19.646	11.400	1.00 20.00	6
	ATOM	2177	С	VAL	В	345	100.096	21.785	12.980	1.00 20.00	. 6
	ATOM	2178	0	VAL	В	345	99.844	22.275	14.085	1.00 20.00	8
	MOTA	2179	N	THR	В	346	100.951	22.335	12.122	1.00 20.00	7
•	ATOM	2180	CA	THR	В	346	101.602	23.610	12.397	1.00 20.00	6
30	ATOM	2181	CB	THR	В	346	103.096	23.593	11.982	1.00 20.00	6
	ATOM	2182	OG1	THR	В	346	103.816	22.688	12.831	1.00 20.00	8
	ATOM	2183		THR			103.707	24.983	12.115	1.00 20.00	6
	ATOM	2184	С	THR			100.810	24.573	11.510	1.00 20.00	6
	MOTA	2185	0	THR			100.950	24.565	10.285	1.00 20.00	8
35	ATOM	2186	N	TRP			99.966	25.385	12.138	1.00 20.00	7
	ATOM	2187	CA	TRP			99.089	26.306	11.425	1.00 20.00	6
	ATOM	2188	CB	TRP			97.941	26.727	12.344	1.00 20.00	6
	ATOM	2189	CG	TRP			97.088	25.594	12.818	1.00 20.00	6
	ATOM	2190	CD2	TRP			95.924	25.071	12.165	1.00 20.00	6
40	ATOM.	2191		TRP			95.436	24.008	12.963	1.00 20.00	6
	ATOM	2192		TRP		_	95.247	25.397	10.983	1.00 20.00	6
	ATOM	2193		TRP			97.259	24.848	13.953	1.00 20.00	6
	ATOM	2194		TRP			96.269	23.893	14.048	1.00 20.00	7
	ATOM	2195		TRP			94.300	23.270	12.616	1.00 20.00	6
45	ATOM	2196		TRP						1.00 20.00	6
•	ATOM	2197	CH2	TRP	В	347	93.654	23.610	11.452	1.00 20.00	6
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50	ATOM	2201	CA	ALA			101.439	29.247	10.822	1.00 20.00	6
	ATOM	2202	СВ	ALA			102.582	29.656	11.761	1.00 20.00	6
	ATOM	2203	C	ALA			101.933	29.277	9,381	1.00 20.00	6
	ATOM	2204	Ö	ALA			101.874	30.323	8.738	1.00 20.00	8
	ATOM	2205	N	ASN			102.411	28.152	8.860	1.00 20.00	7
55	ATOM	2206	CA	ASN			102.411	28.153	7.500	1.00 20.00	6
,,	ATOM	2207	CB	ASN			104.466	28.205	7.569	1.00 20.00	6
	ATOM	2207	CG	ASN			105.058	26.203	8.138	1.00 20.00	6
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	ATOM	2210		ASN			104.445	26.563	7.678	1.00 20.00	7
	111 011	2210	NDZ	UUIN	ب	Jay	100.231	20.303	7.070	1.00 20.00	,

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	MOTA	2211	С	ASN				102.522	26.966	6.634		20.00	6
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	ATOM	2214	CA	LEU		350	٠.	100.776	25.500	5.846	1.00	20.00	6
5	ATOM	2215	CB	LEU	В	350		99.257	25.355	5.973	1.00	20.00	6
	ATOM	2216	CG	LEU	В	350		98.734	24.848	7.316	1.00	20.00	6
	ATOM	2217		LEU	В	350		97.244	25.127	7.418	1.00	20.00	6
	ATOM	2218		LEU				99.030	23.357	7.444	1.00	20.00	6
	ATOM	2219	C	LEU				101.147	25.574	4.365		20.00	6
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10	ATOM	2221	N	HIS		351		101.006	26.744	3.752		20.00	7
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	ATOM	2223	CB	HIS				100.051	29.274	1.618		20.00	6
	ATOM	2224	CG	HIS		351				2.556		20.00	6
. 15	MOTA	2225		HIS				102.001	30.143				.7
	ATOM	2226		HIS				102.072	29.706	0.416		20.00	6
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20	ATOM	2230	0	HIS		351		103.176	26.669	0.832		20.00	8
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	MOTA	2233	CB	GLN	В	352		105.841	27.458	3.819		20.00	6
	ATOM	2234	CG	GLN	В	352		106.395	28.705	3.166		20.00	6
25	ATOM	2235	CD	GLN	В	352		105.930	29.966	3.854	1.00		6
	ATOM	2236	OE1	GLN	В	352·		106.134	30.139	5.053		20.00	8
	ATOM	2237	NE2	GLN	В	.352		105.299	30.854	3.096		20.00	7
	ATOM	2238	С	GLN	В	352		105.478	25.099	3.088	1.00		6
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30	ATOM	2240	N	GLN	В	353		104.514	24.295	3.522		20.00	7
	ATOM	2241	CA	GLN	В	353	•	104.761	22.888	3.777	1.00	20.00	6
	ATOM	2242	CB	GLN	В	353		103.849	22.395	4.900	1.00	20.00	6
	ATOM	2243	CG	GLN	В	353		104.122	23.050	6.240	1.00	20.00	6
	ATOM	2244	CD	GLN	В	353		103.075	22.711	7.281	1.00	20.00	6
35	ATOM	2245		GLN		353		102.627	21.571	7.377	1.00	20.00	8
-	ATOM	2246	NE2	GLN		353		102.690	23.700	8.076	1.00	20.00	7
	ATOM	2247	C	GLN		353		104.507	22.079	2.510	1.00	20.00	6
	ATOM	2248	Ö	GLN		353		103.732	22.490	1.641	1.00	20.00	8
	ATOM	2249	N	THR		354		105.172	20.937	2,401	1.00	20.00	7
40	ATOM	2250	CA	THR		354		104.998	20.071	1.244	1.00	20.00	6
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45		2255	O.	THR				103.745	18.426	2.454		20.00	8
43	ATOM	2256				355		102.741	19.319	0.658		20.00	7
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50	ATOM	2259	CB						20.387	-0.490		20.00	6
50	ATOM	2260	CG			355		101.039		0.766		20.00	
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55	ATOM	2265	CA			356		101.438	14.761	1.573		20.00	6
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	ATOM	2267	CG			356		99.429	15.188	2.737		20.00	6
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                                                                 1.00 20.42
     ATOM
             2295
                   OH2 TIP S
                                6
                                        31.896
                                                13.930
                                                         33.235
                                                                                   s
     ATOM
             2296
                   OH2 TIP S
                                7
                                        50.351
                                                22.781
                                                         28.249
                                                                  1.00 21.14
                                                                                   s
                               . 8
     ATOM
             2297
                   OH2 TIP S
                                        45.246
                                                -0.589
                                                         -0.734
                                                                  1.00 17.74
                                                                                   S
                                      46.249
                                                         -8.523
30
     ATOM
             2298
                   OH2 TIP S
                                                -0.348
                                                                  1.00 21.32
                               11
                                                                                   S
                   OH2 TIP S
                                                                  1.00 21.94
             2299
                                        45.756
                                                         29.680
     MOTA
                               14
                                                11.148
                                                                                   S
     MOTA
             2300
                   OH2 TIP S
                               15
                                        44.273
                                                13.157
                                                         34.592
                                                                 1.00 15.61
                                                                                   s
     ATOM
             2301
                   OH2 TIP S
                               17
                                        53.598
                                                 3.722
                                                         -1.720
                                                                  1.00 21.45
                                                         31.565
             2302
                   OH2 TIP S
                                        46.049
                                                13.087
                                                                 1.00 20.35
     MOTA
                               18
.35
     ATOM
             2303
                   OH2 TIP S
                               19
                                        53.422
                                                22.401
                                                         -3.280
                                                                 1.00 23.26
                                                                                   S
     ATOM
             2304
                   OH2 TIP S
                               20
                                        34.587
                                                 7.922
                                                          5.383
                                                                 1.00 22.58
                                                                                   S
     ATOM
             2305
                       TIP S
                                        45.053
                                                27.379
                                                         19.376
                                                                 1.00 29.60
                   OH2
                               21
                                                                                   S
     MOTA
             2306
                   OH2 TIP S
                               23
                                        28.899
                                                36.416
                                                         28.633
                                                                 1.00.31.68
                                                                                   s
            .2307
                                       35.531
     MOTA
                   OH2 TIP S
                                                11.645
                                                         -8.219
                                                                 1.00 23.45
                               24
                                                                                  S
40
             2308
                   OH2 TIP S
                                        47.364
                                                28.787
                                                         19.612
                                                                 1.00 23.03
     MOTA
                               25
                                                                                  S
     MOTA
             2309
                   OH2 TIP S
                               27
                                       48.859
                                                21.588
                                                        12.634
                                                                 1.00 23.76
     ATOM
             2310
                   OH2 TIP S
                               29
                                       48.805
                                                 8.920
                                                        23.626
                                                                 1.00 22.23
                                                 7.247
                   OH2 TIP S
                                       48.619
                                                                 1.00 21.32
     ATOM
             2311
                               31-
                                                         10.112
                                                                                  S
                   OH2 TIP S
     ATOM
             2312
                               34
                                        44.824
                                                28.720
                                                        15.621
                                                                 1.00 25.27
                                                                                  S
     ATOM
             2313
                   OH2 TIP S
                               35
                                       26.030
                                                12.634
                                                         13.407
                                                                 1.00 21.61
                                                                                  S
    . ATOM
             2314
                   OH2 TIP S
                               36
                                       50.462
                                                19.810
                                                         40.066
                                                                 1.00 25.45
                                                                                  S
     ATOM
             2315
                   OH2 TIP S
                               37
                                       39.631
                                                23.510
                                                         -0.239
                                                                 1.00 30.88
                                                                                  S
                                       44.734
     ATOM
             2316
                   OH2 TIP S
                                                42.655
                                                         10.346
                                                                 1.00 30.84
                               40
                                                                                  S
                   OH2 TIP S
                                       54.653
                                                3.902
                                                         1.503
                                                                 1.00 27.14
     MOTA
             2317
                               41
                                                                                  S
                                       45.693
50
     ATOM
             2318
                   OH2 TIP S
                               45
                                                21.923
                                                         39.754
                                                                 1.00 28.30
                                                                                  S
     ATOM
             2319
                   OH2 TIP S
                               47
                                       47.820
                                                16.413
                                                          7.805
                                                                 1.00 25.73
     ATOM
                                       50.292
             2320
                   OH2 TIP S
                               48
                                                31.412
                                                         29.642
                                                                 1.00 32.79
                                                                                  S
     ATOM
                                       26.056
             2321
                   OH2 TIP S
                               49
                                                16.646
                                                         34.827
                                                                 1.00 29.80
                                                                                  S
     ATOM
             2322
                   OH2 TIP S
                               52
                                       31.714
                                                10.996
                                                         31.855
                                                                 1.00 29.15
                                                                                  S
     ATOM
             2323
                       TIP S
                               53
                                       46.108
                                                23.843
                                                                 1.00 24.21
                   OH2
                                                         -4.299
     ATOM
             2324
                   OH2 TIP S
                               54
                                       37.645
                                                11.206
                                                         34.448
                                                                 1.00 28.56
                                                                                  s
                                                                 1.00 32.08
     ATOM
             2325
                   OH2 TIP S
                               55
                                       26.371
                                                28.513
                                                        12.142
                                                                                  S
                   OH2 TIP S
                              58
                                       33.564
     ATOM
             2326
                                                19.700
                                                         3.483
                                                                 1.00 28.28
                                                                                  S
                                       48.295
     MOTA
             2327
                   OH2 TIP S
                              64
                                                -0.632
                                                        14.280
                                                                 1.00 32.13
```

	ATOM .	2328	OH2 TIP S		40.064	26.036	34.324	1.00 24.17	s
	MOTA	2329	OH2 TIP S		29.570	3.958	14.729	1.00 28.94	S
	MOTA	2330	OH2 TIP S	. —	60.085	11.604	6.814	1.00 38.35	S
	ATOM	2331	OH2 TIP S		39.203	44.403	18.686	1.00 26.61	S
5	MOTA	2332	OH2 TIP S	76	47.312	12.366		1.00 28.51	s
	MOTA	2333	OH2 TIP S	8.0	43.862	33.771	33.329	1.00 28.82	S
	MOTA	2334	OH2 TIP S	81	57.890	13.106	2.128	1.00 40.62	s
	MOTA	2335	OH2 TIP S	82	41.663	34.381	32.043	1.00 19.35	. s
	ATOM	2336	OH2 TIP S	85	50.974	40.331	19.200	1.00 21.14	S
10	MOTA	2337	OH2 TIP S		47.925	-0.832	-6.556	1.00 24.11	S
	MOTA	2338	OH2 TIP S	90	27.231	28.336	33.481	1.00 27.64	s
	MOTA	2339	OH2 TIP S	91	43.651	-7.101	-7.995	1.00 24.33	S
	MOTA	2340	OH2 TIP S	92	49.325	4.387	19.370	1.00 28.02	S
	MOTA	2341	OH2 TIP S		46.231	11.549	33.898	1.00 29.40	S
15	MOTA	2342	OH2 TIP S	94	63.889	24.831	1.168	1.00 26.53	S
	ATOM	2343	OH2 TIP S	96	56.396	4.952	-6.749	1.00 28.00	S
	ATOM	2344	OH2 TIP S	98	35.510	27.986	11.558	1.00 29.24	Ś
	ATOM	2345	OH2 TIP S	100	49.942	24.366	30.265	1.00 31.61	S
	ATOM	2346	OH2 TIP S	101.	56.121	7.113	-8.298	1.00 31.57	S
20	ATOM ·	2347	OH2 TIP S	102	58.318	19.957	-8.378	1.00 26.95	S
	MOTA	2348	OH2 TIP S	103	49.647	22.446	39.624	1.00 40.57	S
	ATOM	2349	OH2 TIP S	104	45.359	7.052	13.052	1.00 26.27	S
	ATOM	2350	OH2 TIP S	105	37.150	32.340	32.346	1.00 34.45	S
	ATOM	2351	OH2 TIP S	107	43.465	40.457	8.240	1.00 40.48	S
25	MOTA	2352	OH2 TIP S	119	36.644	8.257	13.418	1.00 30.70	S
	ATOM	2353	OH2 TIP S	123	41.912	-8.974	-8.264	1.00 26.08	s
	ATOM	2354	OH2 TIP S	124	62.424	15.800	-7.411	1.00 24.08	S
	ATOM	2355	OH2 TIP S	126	37.266	18.656	-9.097	1.00 28.99	S
	ATOM	2356	OH2 TIP S	127	43.129	26.845	14.606	1.00 25.19	S
30	ATOM	2357	OH2 TIP S	128	36.339	32.639	29.802	1.00 29.25	S
	ATOM	2358	OH2 TIP S	130	54.051	14.561	26.498	1.00 33.93	S
	ATOM	2359	OH2 TIP S	131	41.805	-4.242	5.492	1.00 33.72	· s
	ATOM	2360	OH2 TIP S	133	38.873	25.163	36.697	1.00 30.69	s
	ATOM	2361.	OH2 TIP S	134	28.777	8.553	25.307	1.00 31.43	S
35	ATOM	2362	OH2 TIP S	135	53.672	10.546	-12.803	1.00 33.45	S
	ATOM	2363	OH2 TIP S	136	59.892	15.434	11.467	1.00 31.39	S
	ATOM	2364	OH2 TIP S	137	31.040	12.361	35.470	1.00 34.07	S
	ATOM	2365		139	33.489	14.292	-0.598	1.00 40.68	S
	ATOM	2366	OH2 TIP S	140	46.918	8.748	11.662	1.00 29.23	S
40	ATOM	2367	OH2 TIP S	141	46.297	-7.287	-9.196	1.00 42.20	S
	MOTA	2368	OH2 TIP S	142	58.193	6.715	-4.685	1.00 35.48	S
	MOTA	2369	OH2 TIP S	143	44.598	4.435	12.503	1.00 27.68	s
	ATOM	2370	OH2 TIP S	144	27.003	5.999	12.450	1.00 36.30	s
	MOTA	2371	OH2 TIP S	145	43.676	32.852	35.735	1.00 35.70	s
45	MOTA	2372	OH2 TIP S	146	35.783	18.628	36.452	1.00 34.62	s
	MOTA	2373	OH2 TIP S		25.402	4.058	20.638	1.00 45.03	s
	MOTA	2374	OH2 TIP S	148	45.839	35.853	33.724	1.00 35.47	s
	ATOM	2375	OH2 TIP S		22.176	18.976	16.752	1.00 31.87	s
	ATOM	. 2376	OH2 TIP S	150	43.986	33.179	10.162	1.00 37.70	S
50	ATOM	2377	OH2 TIP S	151	50.653	20.347	42.428	1.00 35.80	S
	ATOM	2378	OH2 TIP S	152	47.843	24.314	9.506	1.00 31.05	S
	ATOM	2379	OH2 TIP S		44.693		-14.175	1.00 29.90	s
	ATOM	2380	OH2 TIP S		26.560	36.851	31.684	1.00 49.29	s
	ATOM	2381	OH2 TIP S				-12.951	1.00 29.21	s
55	ATOM	2382	OH2 TIP S		30.432	28.741	12.438	1.00 37.76	s
	ATOM	2383	OH2 TIP S		41.004	20.553	6.423	1.00 39.53	s
	ATOM	2384	OH2 TIP S		49.258	20.069	29.294	1.00 33.97	S
	ATOM	2385	OH2 TIP S		48.082	28.459	16.489	1.00 33.10	s
	MOTA	2386	OH2 TIP S		47.448	18.625	27.683	1.00 34.87	s

	ATOM	2387	OH2 TIP S	162	19.687	20.632	23.411	1.00 35.01	s
	ATOM	2388	OH2 TIP S		32.402	-1.266	22.443	1.00 33.01	S
		2389	OH2 TIP S		39.475	33.468		1.00 37.26	
	MOTA		OH2 TIP S				33.237		S
_	ATOM	2390			44.277	18.950	5.162	1.00 45.14	S
5	ATOM	2391	OH2 TIP S		34.797	30.523	10.736	1.00 47.55	S
	MOTA	2392	OH2 TIP S		46.541		-14.949	1.00 26.54	S
	ATOM	2393	OH2 TIP S		36.333	16.371	1.539	1.00 38.68	S
	MOTA	2394	OH2 TIP S		46.761	38.936	27.403	1.00 34.66	S
	MOTA	2395	OH2 TIP S		24.163	13.264	11.375	1.00 41.23	S
10	ATOM	2396	OH2 TIP S		48.459	15.018	31.951	1.00 38.11	S
	ATOM	2397	OH2 TIP S		34.261	23.193	40.004	1.00 48.96	S
	ATOM	2398	OH2 TIP S	173	45.924	-0.026	13.224	1.00 39.55	
	MOTA	2399	OH2 TIP S	175	41.384	37.389	32.543	1.00 40.74	S
	MOTA	2400	OH2 TIP S	177	49.394	35.312	27.150	1.00 44.33	S
15	ATOM	2401	OH2 TIP S	178	29.066	29.942	34.359	1.00 41.46	s
•	ATOM	2402	OH2 TIP S	180 .	49.354	19.467	7.273	1.00 34.56	S
	ATOM	2403	OH2 TIP S		25.298	17.029	31.863	1.00 47.74	S
	ATOM	2404	OH2 TIP S		37.071	25.027	4.669	1.00 43.87	s
	ATOM	2405	OH2 TIP S		22.581	7.487	18.691	1.00 41.75	S
20	ATOM	2406	OH2 TIP S		32.269	7.011	-1.891	1.00 48.84	s
	ATOM	2407	OH2 TIP S		48.234	0.494	6.833	1.00 48.16	s
	ATOM	2408	OH2 TIP S		20.008	14.658	19.211	1.00 45.27	S
	ATOM	2409	OH2 TIP S		49.341	22.698	42.272	1.00 42.20	S
	ATOM	2410	OH2 TIP S		61.292	18.260	-8.097	1.00 45.21	S
25	ATOM	2411	OH2 TIP S		28.152	10.606	2.819		· s
23	ATOM	2412	OH2 TIP S		25.626	12.619	23.191	1.00 40.38	S
		2412	OH2 TIP S		59.876	11.603	1.216	1.00 34.27	S
	ATOM	2413	OH2 TIP S		57.592			1.00 45.82	S
	MOTA					36.649	-10.646		S
20	ATOM	2415	OH2 TIP S		31.509		21.499	1.00 38.73	
30	ATOM	2416	OH2 TIP S		50.270	-1.543	-6.136	1.00 42.66	S
	ATOM	2417	OH2 TIP S		24.467	8.729	13.088	1.00 42.78	s
	ATOM	2418	OH2 TIP S		38.098	8.699	25.759	1.00 32.80	S
	MOTA	2419	OH2 TIP S		57.831		-13.255	1.00 45.31	s
25	ATOM	2420		201	23.888	22.328	30.524	1.00 37.12	
35	ATOM	2421	OH2 TIP S		47.691	26.068	37.666	1.00 37.92	S
	ATOM	2422	OH2 TIP S		38.653	7.070	29.307	1.00 50.54	S
	ATOM	2423		206	44.424	27.583	2.092	1.00 53.50	S
	MOTA	2424	OH2 TIP S		22.258	2.296	17.948	1.00 47.38	S
	MOTA	2425	OH2 TIP S		19.843	17.943	23.303	1.00 30.36	S
40	MOTA	2426	OH2 TIP S		27.647	11.344	24.681	1.00 31.32	S
	ATOM	2427	OH2 TIP S		37.953	7.817	-9.284	1.00 45.97	S
	ATOM	2428	OH2 TIP S		33.845	34.040	12.124	1.00 38.11	S
	ATOM	2429	OH2 TIP S		58.484	15.269	13.717	1.00 38.26	
	MOTA	2430	OH2 TIP S		48.526	40.920	26.583	1.00 35.23	S
45	MOTA	2431	OH2 TIP S		52.094	21.184	38.122	1.00 29.86	S
	ATOM	2432	OH2 TIP S		36.889	5.881	3.281	1.00 37.63	s
	MOTA	2433	OH2 TIP S	224	47.642	-1.401	-10.684	1.00 34.89	S
	MOTA	2434	OH2 TIP S	226	47.284	2.916	19.133	1.00 34.10	S
	ATOM	2435	OH2 TIP S	227	42.468	4.463	-15.039	1.00 37.98	S
50	ATOM	2436	OH2 TIP S	228	19.169	22.832	21.831	1.00 41.57	S
	ATOM	2437	OH2 TIP S	231	57.592	12.689	14.880	1.00 50.22	. S
	ATOM	2438	OH2 TIP S	232	27.102	9.176	5.655	1.00 40.57	s
	ATOM	2439	OH2 TIP S	233	58.618		-11.925	1.00 50.71	s
	ATOM	2440	OH2 TIP S		22.822	25.342	19.945	1.00 34.93	s
55	ATOM	2441	OH2 TIP S		24.831	32.218	28.901	1.00 37.69	S
	ATOM	2442	OH2 TIP S		20.045	10.774	16.992	1.00 39.57	S
	ATOM	2443	OH2 TIP S		58.019	19.850	15.679	1.00 41.42	S
	ATOM	2444	OH2 TIP S		19.490	20.949	26.114	1.00 34.55	S
	ATOM	2445	OH2 TIP S		61.187	26.377	7.346	1.00 39.68	Ş
	111 011	2447	OHE TIT D		01.10/	20.311	1.540	1.00 33.00	Ļ

	ATOM	2446	OH2 TIP S 241	33.680	38.342 19.389	1.00 48.93	s
	ATOM	2447	OH2 TIP S 242		31.612 10.881	1.00 55.65	S
	MOTA	2448	OH2 TIP S 244	25.872	14.431 30.404	1.00 46.69	S
	ATOM	. 2449	OH2 TIP S 248	37.332	5.849 9.544	1.00 43.81	S
5	ATOM	2450	OH2 TIP S 250	. 39.087	-1.293 -9.655	1.00 42.96	S
	ATOM	2451	OH2 TIP S 258	23.938	30.000 30.010	1.00 38.89	S
	ATOM	2452	OH2 TIP S 259	24.949	29.749 32.578	1.00 40.17	S
	ATOM	2453	OH2 TIP S 260	32.111	17.986 1.918	1.00 48.36	s
	ATOM	2454	OH2 TIP S 266	21.404	12.876 . 25.603	1.00 57.17	·s
10	ATOM	2455	OH2 TIP S 269	35.425	36.767 12.550	1.00 30.70	S
	ATOM	2456	OH2 TIP S 270	52.438	25.529 30.131	1.00 44.85	S
	ATOM	2457	OH2 TIP S 271	53.299	20.156 36.003	1.00 37.15	S
	ATOM	2458	OH2 TIP S 272	50.914	6.919 23.723	1.00 37.13	S
	ATOM	2459	OH2 TIP S 274	31.578	30.795 11.014	1.00 43.29	S
15	ATOM	2460	OH2 TIP S 275	26.341			S
13	ATOM	2461	OH2 TIP S 276		7.243 22.447	1.00 39.40	
	•	2462	OH2 TIP S 276	60.392	18.195 10.235	1.00 37.91	S
	ATOM			47.355	-9.081 -10.821	1.00 48.18	S
	ATOM	2463		41.304	6.175 -16.647	1.00 38.12	S
00	ATOM	2464	OH2 TIP S 282	33.299	21.620 37.881	1.00 46.29	S
20	ATOM	2465	OH2 TIP S 283	56.469	26.112 -8.575	1.00 43.71	S
	ATOM	2466	OH2 TIP S 287	48.382	26.573 7.246	1.00 41.43	S
	ATOM	2467	OH2 TIP S 288	56.240	7.245 - 11.331	1.00 41.79	S
	ATOM	2468	OH2 TIP S 290	49.060	14.978 28.166	1.00 37.03	s
	MOTA	2469	OH2 TIP S 291	37.095	44.270 26.442	1.00 45.08	S
25	ATOM	2470	OH2 TIP S 292	47.814	-0.384 -13.299	1.00 48.60	S
•	MOTA	2471	OH2 TIP S 297	58.081	2.784 - 7.841	1.00 41.89	S
	MOTA	2472	OH2 TIP S 298	36.447	45.321 18.644	1.00 54.91	S
	ATOM	2473	OH2 TIP S 299	49.029	23.328 1.767	1.00 30.55	s
	ATOM	2474	OH2 TIP S 301	24.375	13.771 8.634	1.00 48.47	S
30	MOTA	2475	OH2 TIP S 303	47.904	36.798 28.653	1.00 35.76	s
	ATOM	2476	OH2 TIP S 305	51.156	40.821 27.172	1.00 43.59	S
	ATOM	2477	OH2 TIP S 306	32.943	28.917 35.227	1.00 42.60	S
	ATOM	2478	OH2 TIP S 307	58.462	28.373 6.251	1.00 46.15	S
	ATOM	2479	OH2 TIP S 308	41.964	30.940 36.712	1.00 48.26	s
35	ATOM	2480	OH2 TIP S 313	51.176	-1.922 -3.336	1.00 50.61	s
	ATOM	2481	OH2 TIP S1001	21.319	36.868 23.805	1.00 36.97	S
	ATOM	2482	OH2 TIP S1002	48.880	32.620 27.617	1.00 44.40	S
	ATOM	2483	OH2 TIP S1003	61.880	19.473 11.767	1.00 45.49	S
	ATOM	2484	OH2 TIP S1004	52.770	21.424 26.815	1.00 24.43	S
40	ATOM	2485	OH2 TIP S1005	35.373	29.094 36.197	1.00 35.97	S
	ATOM	2486	OH2 TIP S1006	40.815	-6.636 4.389	1.00 43.15	S
	ATOM	2487	OH2 TIP S1007	44.953	1.286 11.272	1.00 49.45	S
	ATOM	2488	OH2 TIP S1010	21.004	16.168 27.009	1.00 48.51	S
	ATOM	2489	OH2 TIP S1011	47.094	41.786 9.243	1.00 50.10	s
45	ATOM	2490	OH2 TIP S1012	32.479	2.978 14.158	1.00 49.47	S
	ATOM	2491	012 GLC G 1	48.557	11.372 -12.279	1.00 40.72	Ğ
	ATOM	2492	C11 GLC G 1	48.836	12.133 -11.097	1.00 38.05	Ğ
	ATOM	2493	C13 GLC G 1	49.266	13.554 -11.476	1.00 38.09	G
	ATOM	2494	014 GLC G .1	49.559	14.299 -10.292	1.00 33.99	G
50	ATOM	2495	C15 GLC G 1	48.150	14.257 -12.257	1.00 33.33	G
50	ATOM	2496	016 GLC G 1	48.574	15.582 -12.604	1.00 37.32	G
	ATOM	2497	012 GLC G 2	40.114	-6.634 -6.562	1.00 33.74	
	ATOM	2498	C11 GLC G 2	38.967	-6.592 -7.404		G G
	ATOM	2490		37.712		1.00 31.05	
55	ATOM	2500			-6.417 -6.552 -6.406 -7.389	1.00 31.56	G
J.J				36.554	-6.406 -7.389 -5.100 -5.761	1.00 30.70	G
	ATOM	2501		37.792	-5.109 -5.761	1.00 30.03	G
	ATOM	2502	016 GLC G 2	36.609	-4.961 -4.975	1.00 29.66	G
	ATOM	2503	012 GLC G 3	44.030	8.243 -13.470	1.00 37.90	G
	ATOM	2504	C11 GLC G 3	43.950	9.648 -13.690	1.00 38.47	G

	ATOM	2505	C1	3 GL(G	3	42.747	9.974	-14.579	1.00 39.52	_
	ATOM	2506		4 GLC		3	41.551	9 526	-13.942	1.00 39.32	G
	ATOM	2507		5 GLC		3	42.878		-15.934		G
	ATOM	2508		6 GLC				0.200	-15.934	1.00 41.43	G
5						3	41.736		-16.731	1.00 40.78	G
,	ATOM	2509		2 GLC		5.	40.556	1.005	2.289	1.00 45.25	G
	ATOM	2510		1 GLC		5	40.966	2.332	1.960	1.00 40.56	G
	ATOM	2511		3 GLC		5	40.187	3.327	2.814	1.00 40.36	G
	MOTA	2512	01	4 GLC	G	5	38.791	3.169	2.572	1.00 40.71	G
	ATOM	2513	C1!	5 GLC	G	5	40.619	4.751	2.464	1.00 40.04	G
10	MOTA	2514	010	6 GLC	G	5	39.885	5.681	3.256	1.00 36.89	G
	ATOM	2515	012	2 GLC	: G	6	36.951	22.702	40.046	1.00 63.04	G
	ATOM	2516		l GLC		6	37.592	21.583	39.422	1.00 62.46	G
	ATOM	2517		3 GLC		6	38.104	21.978	38.030	1.00 61.14	G
	ATOM	2518		4 GLC		6	39.034	23.054	38.168	1.00 61.14	G
15	ATOM	2519		GLC		6	36.948	22.429			
	ATOM	2520		GLC		6			37.126	1.00 60.51	G
	ATOM	2521		GLC GLC		7	35.992	21.372	36.960	1.00 58.61	G
							37.316	0.281	14.299	1.00 73.45	G
	ATOM	2522		L GLC		7	37.655	-0.758	15.222	1.00 72.78	G
20	ATOM	2523		GLC		7	36.592	-1.856	15.157	1.00 72.98	G
20	ATOM	2524		GLC		7	35.320	-1.299	15.498	1.00 73.88	G _.
	ATOM	2525		GLC		7	36.924	-2.989	16.134	1.00 73.66	G
	ATOM	2526		GLC		7	36.972	-2.493	17.478	1.00 75.38	G
	ATOM	2527	012	GLC	G	8	51.921	21.898	5.908	1.00 62.51	G
	ATOM	2528		LGLC		8	52.447	20.871	5.063	1.00 63.42	G
25	ATOM	2529	C13	GLC	G	8	51.476	20.597	3.908	1.00 64.28	G
	MOTA	2530	014	GLC	G	8	51.297	21.794	3.150	1.00 66.28	G
	ATOM	2531	C15	GLC	G	8	50.121	20.137	4.448	1.00 64.49	G
	ATOM	2532	016	GLC	G	8	49.233	19.886	3.357	1.00 64.01	G
	ATOM	2533	012	GLC	G	10	36.044	37.499	29.523	1.00 56.89	Ğ
30	ATOM	2534	C11	GLC	G	10	35.164	36.645	30.259	1.00 56.97	G
	ATOM	2535		GLC		10	33.849	36.489	29.494	1.00 56.11	.G
	ATOM	2536		GLC		10	33.248		29.308	1.00 56.44	G
	MOTA	2537		GLC		10	32.900	35.580	30.277	1.00 55.84	G
	ATOM	2538		GLC		10	31.674	35.442	29.557	1.00 55.39	G
35	ATOM	2539		ATP		1	46.280	25.658	5.170		
55	ATOM	2540	PG	ATP		1				1.00 51.49	N
	ATOM	2541		ATP			46.464	25.053	3.691	1.00 52.22	N
	ATOM	2542		ATP		1 1	47.406	23.911	3.763	1.00 51.41	N
	ATOM	2543					46.794	26.182	2.784	1.00 52.07	N
40	ATOM			ATP		1	44.976	24.513	3.344	1.00 51.01	N
40		2544	PB	ATP		1	44.560	22.969	3.605	1.00 50.20	, N
	ATOM	2545		ATP		1	43.083	22.898	3.669	1.00 49.41	N
	ATOM	2546		ATP		1	45.345	22.474	4.766	1.00 50.34	N
	ATOM	2547		ATP		1	45.070	22.231	2.255	1.00 47.77	N
4.5	ATOM	2548	PA	ATP		1	45.075	20.613	2.121	1.00 42.84	N
45	MOTA	2549		ATP		1	45.547	20.291	0.754	1.00 43.81	N
•	ATOM	2550		ATP		1	45.807	20.035	3.270	1.00 45.03	N
	MOTA	2551		ATP		1	43.516	20.223	2.245	1.00 41.73	N
	ATOM	2552	C5*	ATP	N	1	42.528	20.925	1.489	1.00 37.57	N
	ATOM	2553	C4*	ATP	N	1	41.127	20.379	1.776	1.00 39.45	N
50	ATOM	2554	04*	ATP	N	1	40.907	19.024	1.279	1.00 37.72	N
	ATOM	2555	C3*	ATP	N	1	40.777	20.321	3.251	1.00 38.48	N
	ATOM	2556		ATP		1	40.360	21.615	3.697	1.00 40.42	N
	ATOM	2557		ATP		ī	39.608	19.374	3.270	1.00 37.58	N
	ATOM	2558		ATP		ī	38.410	20.076	2.924	1.00 37.38	N
55	ATOM	2559		ATP		1	39.939	18.346	2.324	1.00 35.55	
	ATOM	2560	N9	ATP		1	40.628		2.173	1.00 35.55	N
	ATOM	2561	C8	ATP		1	40.028	17.156			N
	ATOM	2562	N7					17.126	3.274	1.00 30.49	N
	ATOM			ATP		1	42.143	15.877	3.667	1.00 29.75	N
	AIOM	2563	C5	ATP	1/1	1	41.088	15.118	3.390	1.00 27.49	N

	ATOM	2564	C4	ATP N	1	40.125	15.925	2.810	1.00 30.02	N
	ATOM	2565	NЗ	ATP N	1	38.937	15.389	2.431	1.00 27.11	N
	MOTA	2566	C2	ATP N	1	38.679	14.085	2.615	1.00 25.62	N
	MOTA	2567	N1	ATP N	1	39.597	13.283	3.175	1.00 21.76	N
5	MOTA	2568	C6	ATP N	1	40.800	13.768	3.571	1.00 23.90	N
	MOTA	2569	N6	ATP N	1	41.698	12.964	4.127	1.00 21.94	N
	MOTA	2570	S	SO4 I	1	58.680	8.493	-0.639	1.00 56.05	I
	MOTA	2571	01	SO4 I	1	57.956	7.875	0.483	1.00 58.83	I
	ATOM .	2572	02	SO4 I	1	57.886	9.607	-1.188	1.00 57.04	I
10	MOTA	2573	03	SO4 I	1	58.906	7.478	-1.683	1.00 57.47	I
-	ATOM	2574	04	SO4 I	1	59.976	9.008	-0.156	1.00 57.51	I
	MOTA	2575	S	SO4 I	2	39.339	4.855	7.057	1.00 84.24	I
	ATOM	2576	01	SO4 I		39.390	6.175	7.711	1.00 85.02	I
	MOTA	2577	02	SO4 I		40.101	4.897	5.797	1.00 84.75	· I
15	ATOM	2578	03	SO4 I	2	37.936	4.506	6.766	1.00 84.94	I
	MOTA	2579	· 04	SO4 I		39.931	3.842	7.954	1.00 84.44	I
	MOTA	2580	S	SO4 I	3	38.987	-2.256	3.310	1.00 58.58	I
	MOTA	2581	01	SO4 I	. 3	37.734	-1.675	3.827	1.00 59.11	I
	ATOM	2582	02	SO4 I	-	39.460	-1.454	2.172	1.00 59.91	I
20	ATOM	2583	03	SO4 I	-	38.743	-3.640	2.866	1.00 60.97	I
	ATOM	2584	04.	SO4 ∙I	3	40.014	-2.260	4.369	1.00 59.58	I
	MOTA	2585	S	SO4 I	4	34.397	5.289	30.981	1.00 64.34	I
	ATOM	2586	01	SO4 I	-	33.627	6.528	30.742	1.00 60.43	I
	· ATOM	2587	02	SO4 · I	4	34.337	4.427	29.782	1.00 60,11	I
25	ATOM	2588	03	SO4 I	4	33.816	4.572	32.133	1.00 64.39	I
	ATOM	2589	04	SO4 I		35.806	5.626	31.277		I
	ATOM	2590	S	SO4 I	5	55.074	-6.984	-3.711	1.00 75.40	I
	ATOM	2591	01	SO4 I	5	54.657	-7.518	-2.399	1.00 74.66	I,
	ATOM	2592	02	SO4 I	5	54.209	-5.845	-4.065	1.00 74.96	I
30	ATOM	2593	03	SO4 I	5	54.950	-8.034	-4.742	1,00 74.22	· I
	MOTA	2594	04	SO4 I	5	56.477	-6.532	-3.633	1.00 75.15	I
	MOTA	2595	02	PO4 P		57.362	24.998	13.149	1.00 66.76	P
	MOTA	2596	03	PO4 P		59.399	26.166	13.761	1.00 66.89	P
	ATOM	2597	04	PO4 P		57.761	25.606	15.462	1.00 67.43	· Р
35	MOTA	2598	01	PO4 P	100	57.264	27.325	13.818	1.00 65.91	P
	ATOM	2599	P	PO4 P	100	57.947	26.025	14.048	1.00 66.69	P
	END			.:						

Example 5: PDK1 fragments

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We produced constructs for expression of different forms of PDK1 in bacteria. The constructs were either in TRC vectors, pET-15b vector and pGEX expression vector to enable the expression of GST fused N-terminally to PDK1. PDK1 expressed from pGEX 51-556 (ie residues 51 to 556 of PDK1) was found to be highly degraded.

PDK1 protein was also expressed with N-terminal His tags from vector TRC comprising PDK1 sequences 51-556, 51-404 and 1-360, or pET15b 51-404 and tested for expression levels and activity. The expression was generally low, around 0.2 mg/L culture. The specific activity was lower than the His-tagged 51-556 protein purified from baculovirus cells. In the case of PDK1 51-404 expressed from pET-15b construct the level of expression turned out to be very variable. This was probably due to instability of the plasmid since we produced evidence that after a growth of 0.2 units of absorbance, (as measured in a spectrophotometer at 600 nm wavelength) the cells growing faster in the culture were actually not harbouring the plasmid with ampiciline resistance. The instability of the plasmid can be due to toxicity produced by basal expression of PDK1. Although production in bacteria was the theoretical best expression system to avoid heterogeneity due to the different extent of phosphorylation of the different phosphorylation sites in hPDK1, it was found that the protein was either degraded, expressed to low levels, had 5 times less specific activity. or was possibly toxic.

The His-tagged purified PDK1 51-556 protein obtained from baculovirus expression system was homogeneous as depicted by the appearance of one band after by SDS-PAGE analysis of a sample.

Nevertheless, the analysis after isoelectric focussing revealed a large smear of protein covering several units of pH. This analysis suggested that the protein was not homogeneous in terms of its isoelectric point, possibly due to the number of phosphorylation sites which were not homogeneously phosphorylated. This protein did not crystallise.

We purified to homogeneity a truncated His-Myc tagged PDK1 (51-404) which lacks the N-terminal 50 residues and the C-terminal 152 residues which include the PH domain. This protein, produced by a baculovirus expression system, had similar characteristics to the full length wild type PDK1 in terms of its activity towards the peptide substrate T308tide, its activation by the peptide PIFtide, and the binding to PIFtide (as analysed by BiaCore). The purified protein was screened for crystallisation conditions using Hampton Research kits (144 different conditions). Crystallisation conditions were screened with two concentrations of PDK1, in the presence or absence of PIFtide, Staurosporine, at 20°C and in the presence of PIFtide at 4°C. No protein crystals were observed after 6 months, suggesting that this construct was not suitable for forming crystals although all other characteristics were similar to wild type protein.

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The His-Myc PDK1 51-404 purified protein was also subjected to protease treatments in order to obtain a protease-insensitive molecule for increasing the chances of obtaining a shorter, stable variant of PDK1. Different protease treatments were tested. Treatment with Glu-C produced a polypeptide of approximately 38 KDa which was stable. This PDK1 protein was active and lacked the His-tag and part of the Myc-tag, and possibly part of the C-terminal residues. This protein was also set up for crystallography screenings. Some crystals were obtained using this preparation after 4 months, but they were not followed up.

A protein kinase corresponding to residues PDk1 51-387 was also produced, in an identical vector to that used to produce the protein PDK1 51-359. Interestingly, this protein was similar to wild type and PDK1 51-404, but had extreme problems for concentration using conventional methods. The protein could not be concentrated further than 2.5 mg/ml, and no crystals were obtained using this construct.

The PDK1 protein that finally crystallised is lacking the first 50 aminoacids and was constructed to end at position 359. This protein was stable in the absence of the PH domain and aminoacids that in hPDK1 link the catalytic domain with the PH domain. The construct PDK1 51-359 was also short enough that no other described phosphorylation sites besides activation loop phosphorylation site 241 were present.

CLAIMS

1. A method for selecting or designing a compound for modulating the activity of phosphoinositide dependent protein kinase 1 (PDK1), the method comprising the step of using molecular modelling means to select or design a compound that is predicted to interact with the protein kinase catalytic domain of PDK1, wherein a three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 is compared with a three-dimensional structure of a compound, and a compound that is predicted to interact with the said protein kinase catalytic domain is selected, wherein the three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 is a three-dimensional structure (or part thereof) determined for a polypeptide consisting of residues equivalent to residues 51 to 359 of full length human PDK1, or a fragment or fusion thereof.

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2. The method of claim 1 wherein the three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 structure is a three-dimensional structure (or part thereof) determined for a polypeptide consisting of residues 51 to 359 of full length human PDK1 or a fusion thereof.

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3. The method of claim 2 wherein the three-dimensional structure (or part thereof) is determined for a polypeptide consisting of residues 51 to 359 of full length human PDK1 and the amino acid sequence Gly-Pro preceding the methionine corresponding to Met51 of human PDK1.

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4. The method of claim 1 wherein the three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 structure is a three-dimensional structure (or part thereof) determined for a polypeptide

consisting of residues 71 to 359 of full length human PDK1 or a fusion thereof.

- 5. The method of any one of the preceding claims wherein the three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 structure is obtainable by X-ray analysis of a crystal obtainable using a mother liquor solution comprising ammonium sulphate.
- 6. The method of claim 5 wherein the mother liquor solution is of pH 7 to 9.
 - 7. The method of claim 6 wherein the mother liquor solution is of pH 8.5.
- 8. The method of any one of claims 5 to 7 wherein the mother liquor solution comprises ATP.
 - 9. The method of any one of claims 1 to 3, 5 to 8 wherein the three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 structure is that represented by the structure co-ordinates shown in Examples 2, 3 or 4, or a structure modelled on such structure co-ordinates.

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10. The method of any one of the preceding claims wherein the molecule is predicted to bind to a region of the structure termed the "PIF binding pocket" (formed by residues including residues Lys115, Ile118, Ile119 on the αB helix, Val124, Val127 on the αC helix and Leu 155 on β -sheet 5 of full length human PDK1, or equivalent residues), the "phosphate binding pocket" (formed by residues including residues Lys76, Arg 131, Thr 148 and Gln150 of full length human PDK1, or equivalent residues) and/or the

α C helix (residues equivalent to 123-136 of full length human PDK1), or interacting regions.

- 11. The method of any of the preceding claims wherein the compound is
 5 for modulating the protein kinase activity of PDK1 towards PKB or other
 PH-domain-comprising/phosphoinositide-binding substrate of PDK1.
 - 12. The method of any one of claims 1 to 10 wherein the compound is for modulating the protein kinase activity of PDK1 towards SGK, S6K or other substrate of PDK1 whose phosphorylation by PDK1 is promoted by phosphorylation of the substrate on the Ser/Thr of the "hydrophobic motif" FXXFS/TY.

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13. A method for selecting or designing a compound for modulating the activity of a hydrophobic pocket (PIF binding pocket)-containing protein kinase having a hydrophobic pocket in the position equivalent to the hydrophobic pocket of human PDK1 that is defined by residues including Lys115, Ile118, Ile119, Val124, Val127 and/or Leu155 of full-length human PDK1 and further having a phosphate binding pocket in the position equivalent to the phosphate binding pocket of human PDK1 that is defined by residues including Lys76, Arg131, Thr148 and/or Gln150, the method comprising the step of using molecular modelling means to select or design a compound that is predicted to interact with the said hydrophobic pocket-containing protein kinase, wherein a three-dimensional structure of a compound is compared with a three-dimensional structure of the said phosphate binding pocket and optionally also the hydrophobic pocket and/or αC helix or region interacting therewith, and a compound that is predicted to interact with the said phosphate binding pocket and optionally

also the hydrophobic pocket and/or αC helix or region interacting therewith, is selected.

- 14. The method of claim 13 wherein the protein kinase is an isoform of Serum and Glucocorticoid stimulated protein kinase (SGK), Protein Kinase B (PKB), p70 S6 kinase, p90 RSK, PKC isoforms (for example PKCα, PKCδ, PKCζ), PRK1, PRK2, MSK1 or MSK2.
- 15. The method of claim 13 or 14 wherein the three-dimensional structure of the said phosphate binding pocket and optionally also the hydrophobic pocket and/or αC helix or region interacting therewith is a structure modelled on the basis of a three-dimensional structure as defined in any one of claims 1 to 9.
- 16. The method of any one of the preceding claims further comprising the step of synthesising, purifying and/or formulating the compound.
 - 17. A method for assessing the activation state of a structure for a protein kinase, wherein the structure is analysed using principle component analysis of the structure co-ordinates.

- 18. The method of claim 17 wherein the activation state of the structure is classified as "open", "closed" or "intermediate".
- 19. A mutated protein kinase, wherein the protein kinase before mutation has a hydrophobic pocket in the position equivalent to the hydrophobic pocket (PIF-binding pocket) of human PDK1 that is defined by residues including Lys115, Ile118, Ile119, Val124, Val127 and/or Leu155 of full-length human PDK1 and further has a phosphate binding pocket in the

position equivalent to the phosphate binding pocket of human PDK1 that is defined by residues including Lys76, Arg131, Thr148 and/or Gln150, and wherein one or more residues equivalent to Ile118, Val124, Val127, Lys76 or Thr148 forming part of the hydrophobic pocket or phosphate binding pocket of the protein kinase is mutated.

- 20. The mutated protein kinase of claim 19 wherein the protein kinase is PDK1.
- 10 21. The mutated protein kinase of claim 19 wherein the protein kinase is SGK, PKB or p70 S6 kinase.
 - 22. The mutated protein kinase of any one of claims 19 to 21 wherein the residue at the position equivalent to residue Lys76 of PDK1 is mutated to an Ala.

- 23. A polynucleotide encoding a mutated protein kinase according to any one of claims 19 to 22.
- 24. A polynucleotide according to claim 23 suitable for expressing a mutated protein kinase according to any one of claims 19 to 22.
 - 25. A host cell comprising a polynucleotide according to claim 23 or 24.
- 26. A method of making a mutated protein kinase according to any one of claims 19 to 22, the method comprising culturing a host cell according to claim 25 which expresses said mutated protein kinase and isolating said mutated protein kinase.
- 30 27. A mutated protein kinase obtainable by the method of claim 26.

- 28. A method of identifying a compound that modulates the protein kinase activity of a protein kinase as defined in claim 19 (for example PDK1), comprising the step of determining the effect of the compound on the protein kinase activity of, or ability of the compound to bind to a mutated protein kinase according to any one of claims 19 to 22, 27.
- 29. The method of claim 28 further comprising the step of determining the effect of the compound on the protein kinase activity of, or ability of the compound to bind to, the protein kinase (for example PDK1) which is not mutated as defined in any one of claims 19 to 22.
- 30. An antibody reactive with the phosphate binding pocket of PDK1 or other protein kinase as defined in claim 19; or an antibody reactive with PDK1 or other protein kinase as defined in claim 19 but not with the said protein kinase mutated at the phosphate binding site, or *vice versa*..
- 31. A method for preparing or selecting an antibody according to claim 30 wherein the antibody is prepared or selected against a said protein kinase (for example PDK1) unmutated at the phosphate binding site and a said protein kinase mutated at the phosphate binding site.
- 32. A kit of parts comprising (1) a mutated protein kinase (for example mutated PDK1) according to any one of claims 19 to 22, 27 (2) the corresponding protein kinase (for example PDK1) which is not mutated as defined in any one of claims 19 to 22.
 - 33. A compound identified or identifiable by any one of claims 1 to 16, 28 or 29.

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- The compound of claim 33 wherein the compound comprises an antibody or RNA molecule.
- A compound according to claim 33 or 34, mutated protein kinase according to any one of claims 19 to 22, 27 or polynucleotide according to claim 23 or 24, for use in medicine.
- 36. Use of a compound, mutated protein kinase or polynucleotide as defined in claim 35 in the manufacture of a medicament for the treatment of a patient in need of modulation of signalling by a protein kinase as defined 10 in claim 19, for example PDK1, SGK, PKB or p70 S6 kinase, for example insulin signalling pathway and/or PDK1/PDK2/SGK/PKB/p70 kinase/PRK2/PKC signalling.
- 37. A method of treating a patient in need of modulation of signalling by a 15 protein kinase as defined in claim 19, for example PDK1, SGK, PKB or p70 S6 kinase. for example insulin signalling pathway PDK1/PDK2/SGK/PKB/p70 S6 kinase/PRK2/PKC signalling, wherein the patient is administered an effective amount of a compound, mutated protein kinase or polynucleotide as defined in claim 35.
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ABSTRACT

A method for selecting or designing a compound for modulating the activity of phosphoinositide dependent protein kinase 1 (PDK1), the method comprising the step of using molecular modelling means to select or design a compound that is predicted to interact with the protein kinase catalytic domain of PDK1, wherein a three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 is compared with a three-dimensional structure of a compound, and a compound that is predicted to interact with the said protein kinase catalytic domain is selected, wherein the three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 is a three-dimensional structure (or part thereof) determined for a polypeptide consisting of residues equivalent to residues 51 to 359 of full length human PDK1, or a fragment or fusion thereof.

A method for selecting or designing a compound for modulating the activity of a hydrophobic pocket (PIF binding pocket)-containing protein kinase having a hydrophobic pocket in the position equivalent to the hydrophobic pocket of human PDK1 that is defined by residues including Lys115, Ile118, Ile119, Val124, Val127 and/or Leu155 of full-length human PDK1 and further having a phosphate binding pocket in the position equivalent to the phosphate binding pocket of human PDK1 that is defined by residues including Lys76, Arg131, Thr148 and/or Gln150, the method comprising the step of using molecular modelling means to select or design a compound that is predicted to interact with the said hydrophobic pocket-containing protein kinase, wherein a three-dimensional structure of a compound is compared with a three-dimensional structure of the said phosphate binding pocket and optionally also the hydrophobic pocket and/or αC helix or region interacting therewith, and a compound that is predicted to interact with the said phosphate binding pocket and optionally

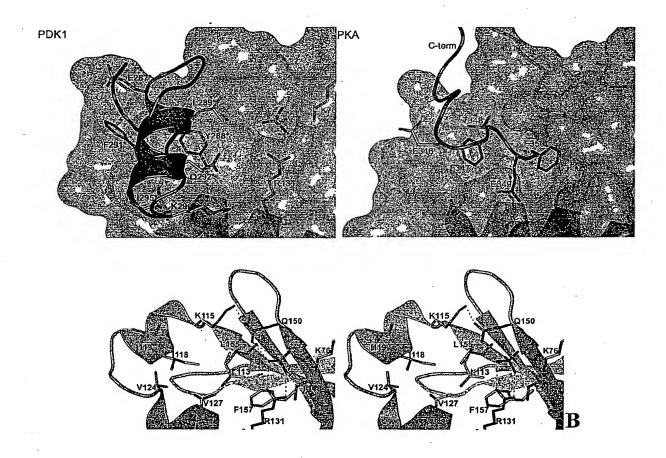
also the hydrophobic pocket and/or αC helix or region interacting therewith, is selected.

FIGURE 1.

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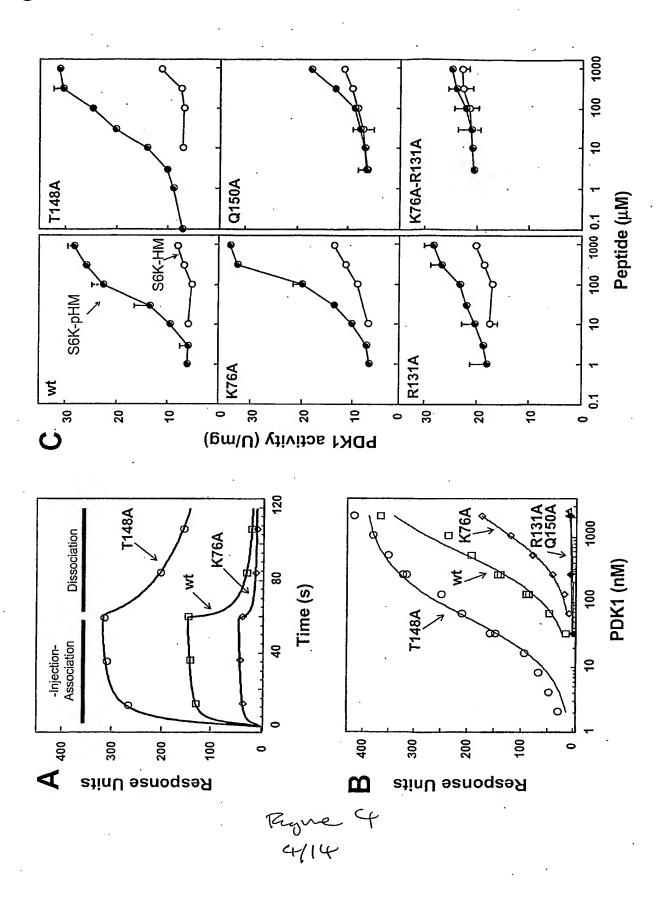
Figure 1 Phosphate-pocket PIF-pocket DFG pS241

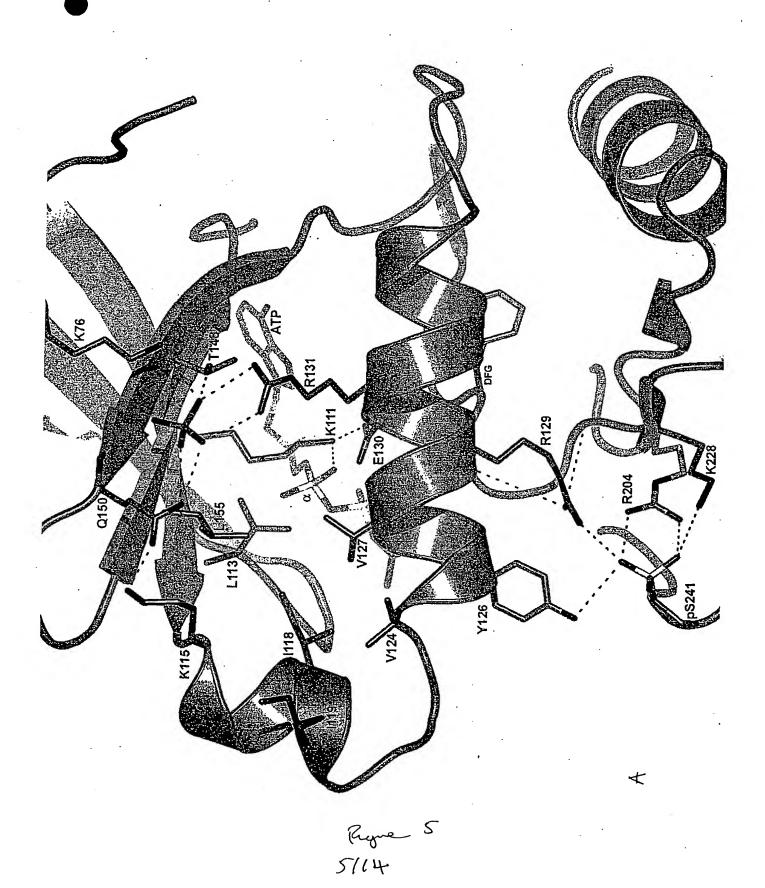


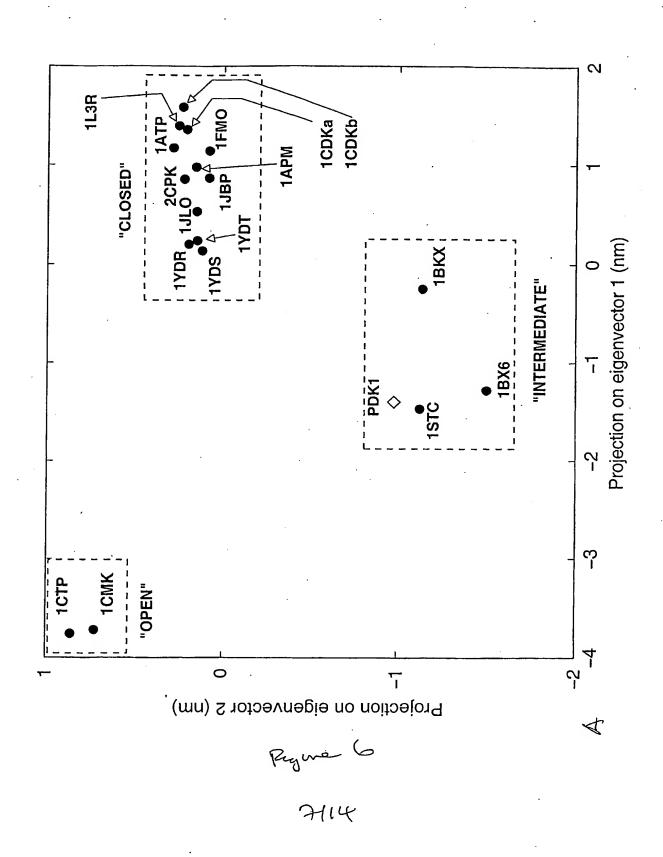
Tyme 2

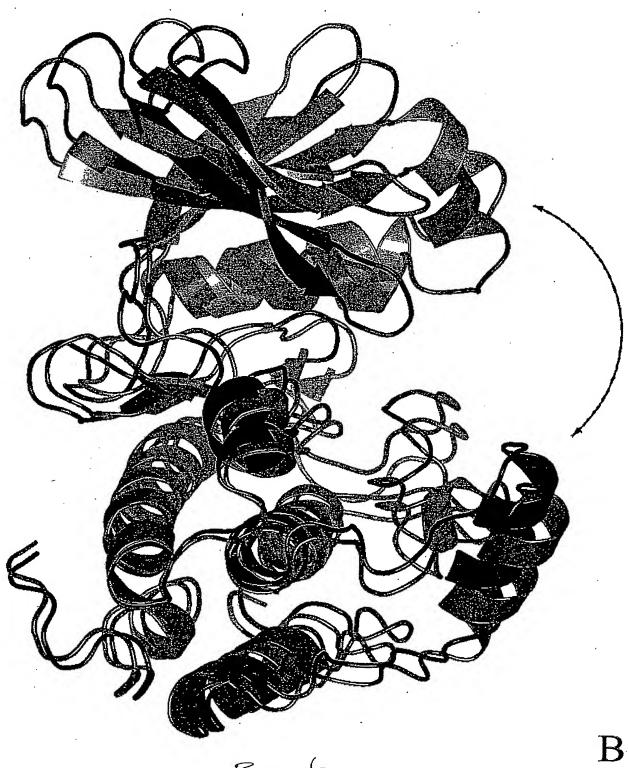
		β1 β2 β3 αB αC
P D K 1	32	U A O D R X K R P W D D R I L L L C I C S B S S T WML A R S B C N I M M M M M M M M M M M M M M M M M M
P D K 1	141	BF VKL X P P P P P P P P P P P P P P P P P P
7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7	211	py kg
1 X X Q Q	281	DO ON SOO DERAGESE YLE SOKTEKLEYD PERSTERSOL KOLDV WORKELGCEEMEGYGPENTUR NON DEKNIRKELGCEEMEGYGPENT DENER
2	351	- HQQ-TPK WIT Y QRKVEA PERP

Ryse 3









Lysits

COMLADRK---GTEELYAIKILKKDVVIQDDDVE-CTMVEKRVLALL--DKPP----FL KVMLAERR---GSDELYAIKILKKDVIVQDDDVD-CTLVEKRVLALG--GRGPGGRPHFL Figure 子(page 1 of 6) (VLLVRLK---KNDQIYAMKVVKKELVHDDEDID-WVQTEKHVFEQA--SSNP--KVLLVRLK---KTDRIYAMKVVKKELVNDDEDID-WVQTEKHVFEQA--SNHP--KVFLVKKISGSDARQLYAMKVLKKATLKVRDRVR--TKMERDILVEVN--H-P-KVFLVRKISGHDTGKLYAMKVLKKATIVQKAKTTEHTRTERQVLEHIR--QSP-KVFQVRKVTGANTGKIFAMKVLKKAMIVRNAKDTAHTKAERNILEEVK--H-P-KVFQVRKVQGTNLGKIYAMKVLRKAKIVRNAKDTAHTRAERNILESVK--H-P-KVFLVKKISGSDARQLYAMKVLKKATLKVRDRVR--TKMERDILVEVN--H-P-KVFLVRKVKGSDAGQLYAMKVLKKATLKVRDRVR--SKMERDILAEVN--H-P-KVFLVRKAGGHDAGKLYAMKVLRKAALVQRAKTQEHTRTERSVLELVR--QAP-KVMLSERK---GTDELYAVKILKKDVVIQDDDVE-CTMVEKRVLALP--GKPP-RVMLVRHO---ETGGHYAMKILNKQKVVKMKQVE-HILNEKRILQAI---DFP-KVLLGELK---GRGEYSAIKALKKDVVLIDDDVE-CTMVEKRVLTLAA--ENP-KVILVREK---ASGKYYAMKILKKEVIIAKDEVA-HTLTESRVLKNT---RHP (VLLSEFR---PSGELFAIKALKKGDIVARDEVE-SLMCEKRILAAVTSAGHP CULLARHK---AEEVFYAVKVLQKKAILKKKEEK-HIMSERNVLLKN--VKHP CVLLAKRK---LDGKFYAVKVLQKKIVLNRKEQK-HIMAERNVLLKN--VKHP KVILVKEK---ATGRYYAMKILKKEVIVAKDEVA-HTLTENRVLQNS KVILVREK---ATGRYYAMKILRKEVIIAKDEVA-HTVTESRVLQNT TVVLAREL---ATSREYAIKILEKRHIIKENKVP-YVTRERDVMSRL 4 He 119 355 628 355 163 165 161 570 80 80. 352 364 258 362 11 257 o70S6Kalpha p70S6Kbeta PKCbetaII **PKCalpha** PKBalpha PKBgamma PKAgamma **PKCgamma** PKCdelta PKBbeta PKCzeta PKCiota PKCbeta p90RSK1 p90RSK2 DORSK3 MSK2 MSK1 PKK2 SGK2 PRK1 SGK1 SGK3

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p70S6Kalpha	215	IYRDLKPENIMLNHQGHVKLTDFGLCKESIHDGT	-VTHTFCGTIEYMAPEILMRSG
p70S6Kbeta	204	IYRDLKPENIMLSSQGHIKLTDFGLCKESIHEGA	-VIHTFCGTIEYMAPEILVRSG
p90RSK1	190	IYRDLKPENILLDEEGHIKLTDFGLSKESIDHEK	-KAYSFCGTVEYMAPEVVNRRG
p90RSK2	190	IYRDLKPENILLDEEGHIKLTDFGLSKESIDHEK	-KAYSFCGTVEYMAPEVVNRRG
p90rsk3	181	IYRDLKPENILLDEEGHIKITDFGLSKEAIDHDK	-RAYSFCGTIEYMAPEVVNRRG
MSK1	174	IYRDIKLENILLDSNGHVVLTDFGLSKEFVADET1	ERAYSFCGTIEYMAPDIVRGGDSG
MSK2	142	IYRDLKLENVLLDSEGHIVLTDFGLSKEFLTEEK1	ERTFSFCGTIEYMAPELIR-SKTG
PKBalpha	271	VYRDLKLENLMLDKDGHIKITDFGLCKEGIKDGA	-TMKTFCGTPEYLAPEVLEDND
. PKBbeta	272	VYRDIKLENLMLDKDGHIKITDFGLCKEGISDGA	-TMKTFCGTPEYLAPEVLEDND
PKBgamma	268	VYRDLKLENLMLDKDGHIKITDFGLCKEGITDAA	-TMKTFCGTPEYLAPEVLEDND
PRK1	737	VYRDLKLDNLLLDTEGYVKIADFGLCKEGMGYGD	-RTSTFCGTPEFLAPEVLTDTS
PRK2	779	VYRDLKLDNLLLDTEGFVKIADFGLCKEGMGYGD	-RTSTFCGTPEFLAPEVLTETS
SGK1	219	VYRDLKPENILLDSQGHIVLTDFGLCKENIEHNS	-TTSTECGTPEYLAPEVLHKQP
SGK3	216	VYRDLKPENILLDSVGHVVLTDFGLCKEGIAISD	-TTTTFCGTPEYLAPEVIRKQP
SGK2	216	IYRDLKPENILLDCQGHVVLTDFGLCKEGVEPED	-TTSTFCGTPEYLAPEVLRKEP
PKCbeta	463	IYRDLKLDNVMLDSEGHIKIADFGMCKENIWDGV	-TTKTFCGTPDYIAPEIIAYQP
.PKCbetaII	463	IYRDLKLDNVMLDSEGHIKIADFGMCKENIWDGV	-TTKTFCGTPDYIAPEIIAYQP
PKCalpha	460	IYRDLKLDNVMLDSEGHIKIADFGMCKEHMMDGV	-TTRTFCGTPDYIAPEIIAYQP
PKCgamma	477	IYRDLKLDNVMLDAEGHIKITDFGMCKENVFPGT	-TTRTFCGTPDYIAPEIIAYQP
PKCzeta	365	IYRDLKLDNVLLDADGHIKLTDYGMCKEGLGPGD	-TTSTFCGTPNYIAPEILRGEE
PKCiota	366	IYRDLKLDNVLLDSEGHIKLTDYGMCKEGLRPGD	-TTSTFCGTPNYIAPEILRGED
. PKCdelta	470	IYRDLKLDNVLLDRDGHIKIADFGMCKENIFGES	-RASTFCGTPDYIAPEILQGLK
PKAgamma	164	IHRDLKPENLLIDQQGYLQVTDFGFAKRVKG	-RTWTLCGTPEYLAPEIILSKG
PDK1	202	IHRDLKPENILLNEDMHIQITDFGTAKVLSPESKQA-RANSFVGTAQYVSPELLT-	-RANSFVGTAQYVSPELLTEKS

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			forth Agnal Camera
p70S6Kalpha	270	HNRAVDWWSLGALMYDMLTGAPPFTGE	NRKKTIDKILKCKLNLPPYLTQEA
p70S6Kbeta	\mathbf{S}	HNRAVDWWSLGALMYDMLTGSPPFTAE	NRKKTMDKIIRGKLALPPYLTPDA
p90RSK1	245	HTQSADWWSFGVLMFEMLTGTLPFQGK	DRKETMTMILKAKLGMPQFLSPEA
p90RSK2	245	HTQSADWWSFGVLMFEMLTGTLPFQGK	DRKETMTMILKAKLGMPQFLSPEA
p90rsk3		HTQSADWWSFGVLMFEMLTGSLPFQGK	DRKETMALILKAKLGMPQFLSGEA
MSK1	232	HDKAVDWWSLGVLMYELLTGASPFTVDG	EKNSQAEISRRILKSEPPYPQEMSALA
MSK2	199	HGKAVDWWSLGILLFELLTGASPFTLEG	ERNTQAEVSRRILKCSPPFPPRIGPVA
PKBalpha	326	YGRAVDWWGLGVVMYEMMCGRLPFYNQD	HEKLPELILMEEIRFPRTLGPEA
PKBbeta	327	YGRAVDWWGLGVVMYEMMCGRLPFYNQD	HERLPELILMEEIRFPRTLSPEA
PKBgamma	323	YGRAVDWWGLGVVMYEMMCGRLPFYNQD	HEKLFELILMEDIKFPRTLSSDA
PRK1	792	YTRAVDWWGLGVLLYEMLVGESPFPGDD	EEEVFDSIVNDEVRYPRFLSAEA
PRK2	834	YTRAVDWWGLGVLIYEMLVGESPFPGDD	EEEVFDSIVNDEVRYPRFLSTEA
SGK1	274	YDRTVDWWCLGAVLYEMLYGLPPFYSRN	TAEMYDNILNKPLQLKPNITNSA
SGK3	271	YDNTVDWWCLGAVLYEMLYGLPPFYCRD	VAEMYDNILHKPLSLRPGVSLTA
SGK2	271	YDRAVDWWCLGAVLYEMLHGLPPFYSQD	VSQMYENILHQPLQIPGGRTVAA
PKCbeta	518	YGKSVDWWAFGVLLYEMLAGQAPFEGED	EDELFQSIMEHNVAYPKSMSKEA
PKCbetaII	518	YGKSVDWWAFGVLLYEMLAGQAPFEGED	EDELFOSIMEHNVAYPKSMSKEA
PKCalpha	515	YGKSVDWWAYGVLLYEMLAGQPPFDGED	EDELFQSIMEHNVSYPKSLSKEA
PKCgamma	_	YGKSVDWWSFGVLLYEMLAGQPPFDGED	EEELFQAIMEQTVTYPKSLSREA
PKCzeta	420	YGFSVDWWALGVLMFEMMAGRSPFDIITI	-DNPDMNTEDYLFQVILEKPIRIPRFLSVKA
PKCiota	421	YGFSVDWWALGVLMFEMMAGRSPFDIVGSSI	YGFSVDWWALGVLMFEMMAGRSPFDIVGSSDNPDQNTEDYLFQVILEKQIRIPRSLSVKA
PKCdelta	525	YTFSVDWWSFGVLLYEMLIGQSPFHGDD	EDELFESIRVDTPHYPRWITKES
PKAgamma	216	YNKAVDWWALGVLIYEMAVGFPPFYADQ	PIQIYEKIVSGRVRFPSKLSSDL
PDK1	259	ACKSSDLWALGCIIYQLVAGLPPFRAGN	EYLIFQKIIKLEYDFPEKFFPKA

p70S6Kalpha	321	RDLLKKLLKRNAASRLGAGPG-DAGEVQAHPFFRHINWEELLARKVEPPFKPLLQSE-
p70S6Kbeta	310	RDLVKKFLKRNPSQRIGGGPG-DAADVQRHPFFRHMNWDDLLAWRVDPPFRPCLQSE-
p90RSK1	296	QSILRMLFKRNPANRLGAGPD-GVEEIKRHSFFSTIDWNKLYRREIHPPFKPATGRP-
p90RSK2	296	QSLLRMLFKRNPANRLGAGPD-GVEEIKRHSFFSTIDWNKLYRREIHPPFKPATGRP-
p90RSK3	287	QSLLRALFKRNPCNRLGAGID-GVEEIKRHPFFVTIDWNTLYRKEIKPPFKPALGRP-
MSK1	287	KDLIQRLLMKDPKKRLGCGPR-DADEIKEHLFFQKINWDDLAAKKVPAPFKPVIRDE-
MSK2	254	QDLLQRLLCKDPKKRLGAGPQ-GAQEVRNHPFFQGLDWVALAARKIPAPFRPQIRSE-
PKBalpha	377	KSILSGLLKKDPKORLGGGSE-DAKEIMOHRFFAGIVWOHVYEKKLSPPFKPQVTSE-
PKBbeta	378	KSLLAGLLKKDPKQRLGGGPS-DAKEVMEHRFFLSINWQDVVQKKLLPPFKPQVTSE-
PKBgamma	374	KSLLSGLLIKDPNKRLGGGPD-DAKEIMRHSFFSGVNWQDVYDKKLVPPFKPQVTSE-
PRK1	843	IGIMRRLLRRNPERRLGSSER-DAEDVKKQPFFRTLGWEALLARRLPPPFVPTLSGR-
PRK2	882	ISIMRRLLRRNPERRLGASEK-DAEDVKKHPFFRLIDWSALMDKKVKPPFIPTIRGR-
SGK1	325	RHLLEGLLQKDRTKRLGAKDDFMEIKSHVFFSLINWDDLINKKITPPFNPNVSGP-
SGK3	322	WSILEELLEKDRONRLGAKEDFLEIQNHPFFESLSWADLVQKKIPPPFNPNVAGP-
SGK2	322	CDLLQSLLHKDQRQRLGSKADFLEIKNHVFFSPINWDDLYHKRLTPPFNPNVTGP-
PKCbeta	569	VAICKGLMTKHPGKRLGCGPE-GERDIKEHAFFRYIDWEKLERKEIQPPYKPKARDK-
PKCbetall	569	VAICKGLMTKHPGKRLGCGPE-GERDIKEHAFFRYIDWEKLERKEIQPPYKPKACG
PKCalpha	266	VSICKGLMTKHPAKRLGCGPE-GERDVREHAFFRRIDWEKLENREIQPPFKPKVCG
PKCgamma	583	VAICKGFLTKHPGKRLGSGPD-GEPTIRAHGFFRWIDWERLERLEIPPFRPRPCG
PKCzeta	478	SHVLKGFLNKDPKERLGCRPQTGFSDIKSHAFFRSIDWDLLEKKQALPPFQPQITDD-
PKCiota	481	ASVLKSFLNKDPKERLGCHPQTGFADIQGHPFFRNVDWDMMEQKQVVPPFKPNISGE-
PKCdelta	576	KDILEKLFEREPTKRLGMTGNIKIHPFFKTINWTLLEKRRLEPPFRPKVKSP-
PKAgamma	267	KDLLRSLLQVDLTKRFGNLRN-GVGDIKNHKWFATTSWIAIYEKKVEAPFIPKYTGP-
PDK1	310	RDLVEKLLVLDATKRLGCEEMEGYGPLKAHPFFESVTWENLHQQTPPKLTAYLPAMSEDD

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p70S6Kalpha	377	EDVSQFDSKFTRQTPVDSPDDSTLSESANQVFLGFTYVAPSVLES-
p70S6Kbeta	366	EDVSQFDTRFTRQTPVDSPDDTALSESANQAFLGFTYVAPSVLDS-
p90RSK1	352	EDTFYFDPEFTAKTPKDSP-GIPPSANAHQLFRGFSFVAITSDDE-
p90RSK2	352	EDTFYFDPEFTAKTPKDSP-GIPPSANAHOLFRGFSFVAITSDDF-
p90RSK3	343	EDTFHFDPEFTARTPTDSP-GVPPSANAHHLFRGFSFVASSLTOEP
MSK1	343	LDVSNFAEEFTEMDPTYSPAALPQSSEKLFOGYSFVAPSILFKR
MSK2	310	LDVGNFAEEFTRLEPVYSPPGSPPGDPRIFOGYSFVAPSTFFF
PKBalpha	433	MECVDSERR
PKBbeta	434	VDTRYFDDEFTAQSITITPPDRYDSLGLLELDORTHFPOFSYSASIRE
PKBgamma	430	PEKYDEDGMDCMDNERPHFPOFSYSASGRE
PRK1	899	TDVSNFDEEFTGEAPTLSPPRDAR-PLTAAEOAAFI,DFDFVAGGC
PRK2	941	EDVSNFDDEFTSEAPILTPPREPR-ILSEEEOEMFRDFDYTADWC
SGK1	380	NDLRHFDPEFTEEPVPNSIGKSPDSVLVTASVKEAAEAFLGFSYAPPT-DSFT
SGK3	377	DDIRNFDTAFTEETVPYSVCVSSDYSIVNASVLEADDAFVGFSYAPPSEDLFT
SGK2	377	ADLKHFDPEFTQEAVSKSIGCTPDTVASSSGASSAFI,GFSYAPFDDTI.D
PKCbeta	625	1
PKCbetail	624	PDQEVIRNID
PKCalpha	621	DIN
PKCgamma	638	RSGENFDKFFTRAAPALTPPDRLVLASIDOADFOGFTYVNPDFVHPD
PKCzeta	532	YGLDNFDTQFTSEPVQLTPDDEDAIKRIDQSEFEGFEYINPLLLSTE
PKCiota	538	FGLDNFDSQFTNEPVQLTPDDDDIVRKIDQSEFEGFEYINPLLMSAE
PKCdelta	628	RDYSNFDQEFLNEKARLSYSDKNLIDSMDQSAFAGFSFVNPKFEHLL
PKAgamma	323	GDASNFDDYEE-EELRISINEK-CAKEFSEF
PDK1	370	EDCYGNYDNLLSQFGCMQVSSSSSHSLSASDTGLPQRSGSNI EQYIHDLDSNSFELDLQ

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